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LOW-STORAGE, EXPLICIT RUNGE-KUTTA SCHEMES FOR THE COMPRESSIBLE NAVIER-STOKES EQUATIONS

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Abstract. The derivation of low-storage, explicit Runge-Kutta (ERK) schemes has been performed in the context of integrating the compressible Navier-Stokes equations via direct numerical simulation. Optimization of ERK methods is done across the broad range of properties, such as stability and accuracy efficiency, linear and nonlinear stability, error control reliability, step change stability, and dissipation/dispersion accuracy, subject to varying degrees of memory economization. Following van der Houwen and Wray, 16 ERK pairs are presented using from two to five registers of memory per equation, per grid point and having accuracies from third- to fifth-order. Methods have been assessed using the differential equation testing code DETEST, and with the 1D wave equation. Two of the methods have been applied to the DNS of a compressible jet as well as methane-air and hydrogen-air flames. Derived 3(2) and 4(3) pairs are competitive with existing full-storage methods. Although a substantial efficiency penalty accompanies use of two- and three-register, fifth-order methods, the best contemporary full-storage methods can be nearly matched while still saving two to three registers of memory.

Key words. explicit Runge-Kutta, low-storage, numerical stability, error control

Subject classification. Applied and Numerical Mathematics

1. Introduction. Direct numerical simulation (DNS) of the compressible Navier-Stokes equations is a means by which researchers may numerically probe the full range of scales in high-speed/fast-time-scale fluid behavior. Compressible DNS seeks to resolve all physically relevant time and length scales associated with phenomena such as turbulence, sound generation, and/or chemical reaction. Resolution of these phenomena is likely to require strict temporal error tolerances. The correspondingly accurate spatial discretizations involving possibly billions of grid points then fill the available memory of the computer. Hence, memory management of the time integrator is an important matter for DNS. The combination of high accuracy and low memory use potential for explicit Runge-Kutta (ERK) schemes makes them ideal for compressible DNS application.

Efforts to reduce computer memory usage during numerical integration of ordinary differential equations (ODEs) have received sporadic attention in the past.[14, 27, 30, 56, 67, 90] For users confronted with severe computer storage constraints, established high-order methods such as the DOPRI5[21] may be prohibitively costly. Currently in the fluid dynamics community, users of ERK methods seeking to reduce memory usage have chosen to implement either a Williamson[87] scheme[25, 32, 64] or a van der Houwen[41, 42] (vdH) method.[4, 81] Williamson and vdH methods are both so called “2N” schemes, where N is the number of equations being integrated times the number of grid points.

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When solving the equation

$$(1.1) \quad \frac{dU}{dt} = F(t, U(t))$$

with an s -stage ERK method, a cavalier implementation requires the storage of the original U -vector, an intermediate U -vector, and all s function evaluations. Williamson implicitly assumes that it is only necessary to be concerned with the memory requirement of a U -vector, what is in effect a dU -vector, and that the memory requirement of F is inconsequential. Loosely, he implements the strategy over a single intermediate stage as

$$(1.2) \quad \begin{aligned} dU^{(j)} &= A_j dU^{(j-1)} + (\Delta t) F^{(j)} \\ U^{(j)} &= U^{(j-1)} + B_j dU^{(j)}, \end{aligned}$$

where A_j and B_j are functions of the standard Butcher coefficients, $F^{(j)}$ and $U^{(j)}$ are the j^{th} intermediate values of the function evaluation and the integration vector, and Δt is the step size. Note that U , dU , and F must be stored. Unless work is done in a piecemeal fashion, three storage registers per variable will be required for the Williamson scheme. These methods have been referred to as 2N schemes.

Wray[90], employing van der Houwen's technique, places a set of conditions the scheme must satisfy that are more restrictive than Williamson's. Van der Houwen and Wray devise a scheme where information alternates between the two available storage registers at each successive ERK stage. The procedure is loosely written over two intermediate stages as

$$(1.3) \quad \begin{aligned} \text{(Register 1)} \quad & U^{(j+1)} = X^{(j)} + (a_{j+1,j}) \Delta t F^{(j)} \\ \text{(Register 2)} \quad & X^{(j+1)} = U^{(j+1)} + (b_j - a_{j+1,j}) \Delta t F^{(j)} \\ \text{(Register 2)} \quad & U^{(j+2)} = X^{(j+1)} + a_{j+2,j+1} \Delta t F^{(j+1)} \\ \text{(Register 1)} \quad & X^{(j+2)} = U^{(j+2)} + (b_{j+1} - a_{j+2,j+1}) \Delta t F^{(j+1)}. \end{aligned}$$

By overwriting, the U , F , and X vectors never fully coexist. The symbols a_{ij} and b_j are the ordinary Butcher coefficients of the scheme. The X vector may be thought of as a vehicle to bring information from previous stages into the current stage. To distinguish these methods from the Williamson class of 2N schemes, we will refer to them as 2R schemes.

The primary difference in philosophy between the two methods is that in the vdH scheme, during the function evaluation, the previous solution vector is overwritten. Clearly there will be cases where this is not acceptable. Compressible DNS provides a situation where this method may be profitably utilized. This circumstance occurs because the U -vector contains, principally, variables which are the products of variables needed to evaluate the flux terms. Consequently, the U -vector must be decomposed into other variables, leaving the U -vector itself disposable. Both Williamson (2N) and vdH (2R) schemes may be easily generalized to accommodate more than two storage registers (N or R). We make no claim that these two strategies are the only viable ones. We do suggest, however, that the vdH methodology is extremely aggressive in its conservation of computer memory usage.

In the pursuit of computer memory use reduction, the first casualty is the retention of the U -vector at the beginning stage. Error control, in the more traditional sense, becomes impossible. A rejected step (such as violation of the error tolerance) cannot be restarted from $U^{(n)}$ because with a 2N or 2R scheme, $U^{(n)}$ is no longer available. Instead, allotting one additional register for an error estimate, one may monitor the error

occurring at each step and determine an appropriate next step. Including yet another register, $U^{(n)}$ could be retained so that action could be taken on a step which exceeds the predetermined error bound. This additional register approach, however, undermines the fundamental premise of this work and should not be used unless all other approaches fail. Schemes in this paper that can be used in error monitoring/control mode are designated 2R+, etc., schemes because, if used in this mode, they require extra storage. Details of this implementation are contained in Appendix A. If overwriting is impossible, then the implementation must be modified and an extra storage register will be required.

The goal of this paper is to derive broadly optimized, minimal-storage (2R+, 3R+, 4R+, and 5R+) ERK schemes based on only the vdH methodology and to explain how they are implemented. Choices are offered for storage reduced methods that address the needs of stability efficiency, accuracy efficiency, linear stability, nonlinear stability, dissipation and dispersion minimization, time-step/error control, and step-control stability. Invariably users will investigate physical phenomena that require different integrator properties, different error tolerances, and have different computer memory allocations. Hence, many good schemes are presented along with a rational basis by which to choose a scheme depending on one's needs. Based on the existing literature, the fluid dynamics community has been the largest customer for these low-storage schemes. For this reason (as well as personal research interests), optimization of ERK schemes is made with an eye towards the Navier-Stokes equations. Flows which are strongly viscous or chemically stiff may not be good candidates for these explicit methods. In addition, integrating the differential-algebraic equations arising from the discretization of the incompressible or low Mach number equation set with an ODE-ERK method must be done with great caution so as to avoid drift-off and/or order reduction.

A recurring criticism that accompanies use of high-order ERK schemes for discretized partial differential equations (PDEs) is the boundary "order reduction" phenomenon.[1, 13, 47, 49, 61, 66] Without proper care, order reduction occurring at the spatial boundaries can dominate the solution accuracy throughout the entire domain. The impact of the order reduction becomes more pronounced with increasing temporal accuracy. As such, the new schemes presented in this paper will be more susceptible to this problem than either Williamson's or Wray's third-order schemes.

A second concern is that Runge-Kutta methods may seek out spurious fixed points of the differential equations being integrated. Methods exhibiting this behavior are called irregular.[2, 38, 78, 80, 83] All ERK methods greater than first-order accurate are irregular. We rely on error control and the fact that many equations are being integrated simultaneously to avoid spurious fixed points.

Finally, we largely forsake aesthetic or "nice" coefficients (ones with simple, rational numbers) because the benefit from using a substantially more efficient integrator over hundreds of simulations, each taking tens or hundreds of hours, far outweighs the inconvenience of typing in twenty or so complicated coefficients correctly. Most solutions that are presented within this paper have been found numerically with established mathematical software.[18, 28, 29, 58, 88] Attempts were made to solve for schemes symbolically, but it was found that the assumption of various $a_{ij} = b_j$ quickly made matters intractable because the equations of condition become algebraically nonlinear in the b_i 's. Scheme coefficients are given to at least 25 digits of accuracy.

Some ERK background is necessary to facilitate a discussion on the optimization of accuracy efficiency, stability efficiency, error control reliability, step-control stability, linear stability, nonlinear stability, and dispersion and dissipation error within the context of storage reduction in later chapters. This will be done in sections 1 and 2. Two-register schemes will be reviewed in section 3 while three-, four-, and five-register schemes will be considered in sections 4, 5, and 6. Merits of the low-storage schemes are discussed in section

7, and comparisons are made with more traditional, full-storage ERK methods. In section 8, conclusions are drawn as to the utility of the various schemes. Appendices listing an implementation strategy and the relevant equations of constraint are also included.

2. Background. We cannot hope to review the extensive body of Runge-Kutta literature germane to integrating the Navier-Stokes equations. Therefore we tersely describe only those areas of literature that are crucial to the development of the new schemes being presented. For further details, appropriate references are provided.

The compressible Navier-Stokes equations constitute a coupled set of partial differential equations that may be spatially discretized into a set of coupled ODEs with finite-difference techniques by the method of lines. We are concerned with the numerical solution of the initial value problem

$$(2.1) \quad \frac{dU}{dt} = F(t, U(t)), \quad U(a) = U_0, \quad t \in [a, b],$$

where $U = (\rho, \rho \mathbf{u}, \rho e_0, \rho Y_i)^T$ is a function of the fluid density, ρ , velocity vector, \mathbf{u} , total specific internal energy, e_0 , and species mass fraction, Y_i . F contains the inviscid, viscous, reactive, and, possibly, body force terms of the compressible Navier-Stokes equations.

Temporal discretization of the Navier-Stokes equations can be made with an s -stage ERK scheme, which may include an embedded error control scheme within the s -stage procedure. The implementation over a time step Δt , from time level $t^{(n)}$ to time level $t^{(n+1)}$, is accomplished as

$$(2.2) \quad \begin{aligned} F^{(i)} &= F^{(i)}(t^{(i)}, U^{(i)}), \quad U^{(i)} = U^{(n)} + \Delta t \sum_{j=1}^{i-1} a_{ij} F^{(j)}, \quad t^{(i)} = t^{(n)} + c_i \Delta t, \\ U^{(n+1)} &= U^{(n)} + \Delta t \sum_{j=1}^s b_j F^{(j)}, \quad \hat{U}^{(n+1)} = U^{(n)} + \Delta t \sum_{j=1}^s \hat{b}_j F^{(j)}, \end{aligned}$$

where $U^{(n)} = U^{(1)} = U(t^{(n)})$ and $U^{(n+1)} = U(t^{(n)} + \Delta t)$ are the solutions at time levels n and $n+1$ of order $q = p + 1$ and $\hat{U}^{(n+1)}$, the U -vector associated with the embedded scheme, is of order p . The particular Butcher coefficients a_{ij} , b_i , \hat{b}_i , and c_i of the respective schemes are constrained by certain equations of condition, a short list of which may be found in appendix B. In reading these conditions we remark that for a q^{th} -order ERK, the k^{th} equation of condition may be considered as [9, 35]

$$(2.3) \quad \tau_k^{(q)} = \frac{1}{\sigma} \Phi_k^{(q)} - \frac{\alpha}{q!},$$

which defines $\Phi_k^{(q)}$, a scalar sum of Butcher coefficient products that will appear throughout this paper. Both α and σ vary with q and k . The $\hat{\tau}_k^{(q)}$ conditions are identical to $\tau_k^{(q)}$ conditions with \hat{b}_i replacing b_i . We assume that the standard row-sum condition applies: $c_i = \sum_{j=1}^s a_{ij}$. Extensive discussions of explicit Runge-Kutta methods may be found in the literature. [9, 21, 24, 35, 54, 69] Our style in this paper closely follows Dormand et al. [20] Schemes will be referred to as RKq(p)s[rR,nN+]X{ q_{disp}, q_{diss} }, where q is the order of the main scheme, p is the order of the embedded scheme, s is the number of stages, r/n is the number of registers used (vdH/Williamson), $+$ denotes that extra storage registers will be needed for error monitoring/control, X denotes either C (linear stability-error compromise), S (maximum linear stability), F (FSAL - first same as last), M (minimum truncation error), N (maximum nonlinear stability - contractive), or P (minimum phase error), and for "P" methods, q_{disp} and q_{diss} are the respective dispersion and dissipation orders of accuracy.

2.1. Error and Error Control. Error in a q^{th} -order explicit Runge-Kutta scheme may be quantified in a general way by taking the L_2 and L_∞ principal error norms,[62, 86]

$$(2.4) \quad A^{(q+1)} = \|\tau^{(q+1)}\|_2 = \sqrt{\sum_{j=1}^{n_{q+1}} \left(\tau_j^{(q+1)}\right)^2}, \quad A_\infty^{(q+1)} = \|\tau^{(q+1)}\|_\infty = \text{Max}\{|\tau_j^{(q+1)}|\},$$

where $\tau_j^{(q)}$ are the $n_q = \{1, 1, 2, 4, 9, 20, 48, 115, 286\}$ error coefficients associated with order of accuracy $q = \{1, 2, 3, 4, 5, 6, 7, 8, 9\}$. For embedded schemes of accuracy p , additional definitions are useful, such as

$$(2.5) \quad \hat{A}^{(p+1)} = \|\hat{\tau}^{(p+1)}\|_2 = \sqrt{\sum_{j=1}^{n_{p+1}} \left(\hat{\tau}_j^{(p+1)}\right)^2},$$

$$(2.6) \quad B^{(p+2)} = \frac{\hat{A}^{(p+2)}}{\hat{A}^{(p+1)}} = \frac{\|\hat{\tau}^{(p+2)}\|_2}{\|\hat{\tau}^{(p+1)}\|_2} = \frac{\sqrt{\sum_{j=1}^{n_{p+2}} \left(\hat{\tau}_j^{(p+2)}\right)^2}}{\sqrt{\sum_{j=1}^{n_{p+1}} \left(\hat{\tau}_j^{(p+1)}\right)^2}},$$

$$(2.7) \quad C^{(p+2)} = \frac{\|\hat{\tau}^{(p+2)} - \tau^{(p+2)}\|_2}{\|\hat{\tau}^{(p+1)}\|_2} = \frac{\sqrt{\sum_{j=1}^{n_{p+2}} \left(\hat{\tau}_j^{(p+2)} - \tau_j^{(p+2)}\right)^2}}{\sqrt{\sum_{j=1}^{n_{p+1}} \left(\hat{\tau}_j^{(p+1)}\right)^2}},$$

$$(2.8) \quad D = \text{Max}\{|a_{ij}|, |b_i|, |\hat{b}_i|, |c_i|\},$$

$$(2.9) \quad E^{(p+2)} = \frac{A^{(p+2)}}{\hat{A}^{(p+1)}} = \frac{\|\tau^{(p+2)}\|_2}{\|\hat{\tau}^{(p+1)}\|_2} = \frac{\sqrt{\sum_{j=1}^{n_{p+2}} \left(\tau_j^{(p+2)}\right)^2}}{\sqrt{\sum_{j=1}^{n_{p+1}} \left(\hat{\tau}_j^{(p+1)}\right)^2}}.$$

One may also consider $\hat{A}_\infty^{(p+1)}$, $B_\infty^{(p+2)}$, $C_\infty^{(p+2)}$, and $E_\infty^{(p+2)}$. All embedded schemes considered here are applied in local extrapolation mode; i.e., the solution is advanced with the higher - order formula. For a given order of accuracy, one strives to reduce $A^{(q+1)}$ to as small number as possible. Both $B^{(p+2)}$ and $C^{(p+2)}$ should be of order unity. The maximum magnitude of any of the Butcher coefficients, D , should be small, but may approach 20 in some high-quality pairs.[72] Shampine[68] recommends $B^{(p+2)} < 1.5$ and $E^{(p+2)} < 0.5$. Although these error measures are independent of the equations being integrated and hence only an approximate error metric, they will be used to select the “best” scheme. Verner[85] points out that strictly relying on only $A^{(q+1)}$, $B^{(p+2)}$, and $C^{(p+2)}$ may not be adequate to distinguish among several good schemes. He also presents $A_\infty^{(q+1)}$, $\hat{A}_\infty^{(p+1)}$, $B_\infty^{(p+2)}$, and $C_\infty^{(p+2)}$. In another paper, Verner[84] recommends that $\tau^{(q+1)}$ should generally not vanish. Although not as frequently mentioned as the above parameters, the ratio of $A^{(q+2)}/A^{(q+1)}$ is sometimes controlled. For 5(4) pairs, Sharp and Smart[72] choose 5/2, Bogacki and Shampine[6] limit it to 10, while Papakostas and Papageorgiou[60] use 25. The risk of allowing $A^{(q+2)}/A^{(q+1)}$ to grow too large is that the error controller may become less reliable at lax tolerances. Additionally, we require that all $\hat{\tau}_j^{(p+1)} \neq 0$ to avoid a defective embedded method, i.e., $R_z = 0$. The stability domain of the embedded method is designed to be nearly as large as that of the main method to avoid instability in the embedded method at large step sizes.

FSAL techniques, where $a_{sj} = b_j$, allow for the use of not only all function evaluations during an effectively s -stage computation, but also use $F^{(n+1)}$. After $U^{(n+1)}$ and $F^{(n+1)}$ are evaluated, $\hat{U}^{(n+1)}$ is computed with $s + 1$ function evaluations. The principal motivation for doing this is that it allows more latitude in the design of the method and usually results in better schemes. The high stage numbers found

in low-storage schemes make FSAL relatively less advantageous. Dense output via Runge-Kutta triples is forsaken here because there is little apparent interest within the DNS user community for such a feature. It may, however, find use if users seek global error estimates.[3] Pseudosymplectic or low-drift methods are also forsaken.

2.2. Linear Stability. The stability function[36] for ERK methods is given by

$$(2.10) \quad R(z) = \text{Det} [\delta_{ij} - (a_{ij} - e_i b_j)z],$$

$$(2.11) \quad = 1 + \Phi_1^{(1)}z + \Phi_1^{(2)}z^2 + \Phi_2^{(3)}z^3 + \Phi_4^{(4)}z^4 + \Phi_9^{(5)}z^5 + \cdots + \Phi_{n_s}^{(s)}z^s,$$

with $\mathbf{e} = \{1, 1, \dots, 1\}$, δ_{ij} is the identity matrix, $\Phi_{n_i}^{(i)}$ are the “tall trees,” and z contains information (eigenvalues) describing the equations being integrated. It is convenient in fluid dynamics to consider linear stability in the context of the prototypical, one-dimensional, convection-diffusion equation

$$(2.12) \quad \frac{\partial U}{\partial t} = \left\{ -a \frac{\partial}{\partial x} + \alpha_v \frac{\partial^2}{\partial x^2} \right\} U,$$

where a is a convection or sound velocity and α_v is a diffusivity[48] (mass, momentum, or energy). Other studies of stability of ERK methods applied to the compressible Navier-Stokes equations have been conducted by Sowa[75] and Müller.[59] If the spatial derivatives are considered as high-order, centered, finite-difference operators then the Fourier image of the convection-diffusion equation becomes

$$(2.13) \quad z = -\lambda \Psi + \lambda_v \Psi^2,$$

$$(2.14) \quad \Psi = \frac{i [2a \sin(\xi) + 2b \sin(2\xi) + 2c \sin(3\xi) + \cdots]}{[1 + 2\alpha \cos(\xi) + 2\beta \cos(2\xi) + \cdots]}.$$

In this expression $\lambda = \frac{a\Delta t}{\Delta x}$ and $\lambda_v = \frac{\alpha_v \Delta t}{(\Delta x)^2}$ are the inviscid and viscous CFL numbers, Δx is the local spatial grid spacing, Δt is the magnitude of one time step, $0 \leq \xi \leq \pi$ is the spatial wavenumber, Ψ is the Fourier image of the first derivative operator, and $\{a, b, c, \alpha, \beta\}$ are coefficients of the derivative operator used in evaluating the convection-diffusion equation. As the “compact” sixth-order derivative operator is popular in compressible DNS, these last coefficients will be set to $\{7/9, 1/36, 0, 1/3, 0\}$. [48]

A stable method has $|R(z)| < 1$ at a particular value of z or for all wavenumbers at the pair (λ, λ_v) . This requirement is necessary but may not be sufficient.[33, 50, 65] Unlike many contemporary ERK pairs, imaginary axis stability is a high priority to the methods designed in this paper. The derived linear stability domains, in terms of (λ, λ_v) , are a strong function of which derivative operator is chosen. Reducing truncation error of the spatial derivative operator reduces the extent of the linear stability regime. Use of the corresponding second derivative operator rather than repeated use of the first derivative operators for the viscous terms reduces the maximum viscous CFL number. Nevertheless, determining linear stability as previously described gives results representative of a broad class of numerical methods used for DNS of compressible flows.

2.3. Step Control Stability. We consider two step-size control strategies:[34, 36, 37]

$$(2.15) \quad (\Delta t)^{(n+1)} = \kappa (\Delta t)^{(n)} \left\{ \frac{\epsilon}{\|\delta^{(n+1)}\|_\infty} \right\}^\alpha,$$

$$(2.16) \quad (\Delta t)^{(n+1)} = \kappa (\Delta t)^{(n)} \left\{ \frac{\epsilon}{\|\delta^{(n+1)}\|_\infty} \right\}^\alpha \left\{ \frac{\|\delta^{(n)}\|_\infty}{\epsilon} \right\}^\beta,$$

where ϵ is some chosen integration error tolerance, $\kappa \approx 0.9$, and $\delta^{(n+1)} = U^{(n+1)} - \hat{U}^{(n+1)}$. The first and most common method, Eq. (2.15) is an example of an integral feedback (I-) controller. The second, more

sophisticated, Eq. (2.16) adds a proportional feedback component and is called a PI-controller. Following Hairer and Wanner,[36] we define

$$(2.17) \quad R(z) = 1 + \sum_{i=1}^s \Phi_{n_i}^{(i)} z^i, \quad E(z) = \sum_{i=p+1}^s \left(\Phi_{n_i}^{(i)} - \hat{\Phi}_{n_i}^{(i)} \right) z^i, \quad u = \Re \left[\frac{R'(z)z}{R(z)} \right], \quad v = \Re \left[\frac{E'(z)z}{E(z)} \right],$$

as well as the matrices

$$(2.18) \quad C = \begin{pmatrix} 1 & u \\ -\alpha & (1 - \alpha u) \end{pmatrix}, \quad \tilde{C} = \begin{pmatrix} 1 & u & 0 & 0 \\ -\alpha & (1 - \alpha u) & \beta & \beta v \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}.$$

In the case of the C -matrix corresponding to Eq. (2.15), $\alpha = (p+1)^{-1}$. For \tilde{C} corresponding to Eq. (2.16), we set $\alpha = 0.7/p$ and $\beta = 0.4/p$ where p is the order of the embedded method. If at the regions where $|R(z)| = 1$ the spectral radius of C or \tilde{C} is less than unity, then the step-size control mechanism is said to be SC-stable. As DNS runs are often made near the linear stability limits of the integrator, step-size change oscillations may result and give rise to a rapid accumulation of global error during oversteps. Still more involved would be a PID-controller, which we do not use. The PID-controller is obtained by multiplying the RHS of Eq. (2.16) by $\{\epsilon/||\delta^{(n-1)}||_\infty\}^\gamma$ and creating a 6×6 matrix \check{C} which has the elements $\check{C}_{ij} = \check{C}_{ij}, i, j = 1, 2, 3, 4$, $\check{C}_{25} = -\gamma$, $\check{C}_{26} = -\gamma v$, and $\check{C}_{53} = \check{C}_{64} = 1$, with all remaining elements being zero.

2.4. Dispersion and Dissipation Error. Dispersion and dissipation of ERK methods[10, 44, 45] may be considered by taking the derivative of $U = e^{i\omega t}$ with respect to time, $dU/dt = i\omega U$, where ω is a temporal wavenumber (frequency). The stability function for this ODE has the argument $i\nu$ where $\nu = \omega(\Delta t)$. An ERK method where \mathcal{R} and \mathcal{I} , respectively, are the real and imaginary parts of $R(i\nu)$ is said to be dispersive of order q_{disp} and dissipative of order q_{diss} if

$$(2.19) \quad \phi(\nu) = \nu - \arg(R(i\nu)) = \nu - \arctan\left(\frac{\mathcal{I}}{\mathcal{R}}\right) = \sum_{j=0}^{2j+1} \phi_{2j+1} \nu^{2j+1} = O(\nu^{q_{\text{disp}}+1}),$$

$$(2.20) \quad \alpha(\nu) = 1 - |R(i\nu)| = 1 - \sqrt{\mathcal{R}^2 + \mathcal{I}^2} = \sum_{j=0}^{2j} \alpha_{2j} \nu^{2j} = O(\nu^{q_{\text{diss}}+1}).$$

Hence $R(i\nu) = \mathcal{R} + i\mathcal{I} = (1 - \alpha(\nu)) e^{i(\nu - \phi(\nu))}$. Some authors refer to the phase-lag order of the method, which, in our notation, would be $(q_{\text{disp}}, q_{\text{diss}} - 1)$. Control of both spatial and temporal dissipation and dispersion in acoustics applications has employed ERK methods satisfying only quadrature[46, 92] and subquadrature[93] order conditions. Applied to nonlinear problems like the Navier-Stokes equations, these methods will generally not exceed second- and third-order accuracy, respectively.

2.5. Nonlinear Stability. Nonlinear stability of Runge-Kutta methods[53] focuses on the discrete analog to dissipativity of $F(t, U(t))$ in some given norm,

$$(2.21) \quad \|\tilde{U}(t + \Delta t) - U(t + \Delta t)\| \leq \|\tilde{U}(t) - U(t)\|,$$

where \tilde{U} is a perturbed approximation to U and $F(t, U(t))$ belongs to any one of the four function classes: linear (\mathcal{L}) or nonlinear (\mathcal{F}) and dissipative in an inner product or maximum norm. For ERK methods,[15, 52, 53, 55, 91] the dissipativity criterion is replaced with the so-called circle-condition, and maximum step-sizes are related to a contractivity threshold: the largest possible step-size that ensures $\|\tilde{U}^{(n+1)} - U^{(n+1)}\| \leq$

$||\tilde{U}^{(n)} - U^{(n)}||$. A radius of conditional or circular contractivity for the four function classes may be denoted $r_{\mathcal{F}_\infty}$, $r_{\mathcal{L}_\infty}$, $r_{\mathcal{F}_2}$, $r_{\mathcal{L}_2}$ where $r_{\mathcal{F}_\infty} \leq r_{\mathcal{L}_\infty} \leq r_{\mathcal{L}_2}$ and $r_{\mathcal{F}_\infty} \leq r_{\mathcal{F}_2} \leq r_{\mathcal{L}_2}$. We will call a method (conditionally) contractive if at least $r_{\mathcal{F}_2} > 0$.

Kraaijevanger[52] (\mathcal{F}_∞) and Dahlquist and Jeltsch[16] (\mathcal{F}_2) have shown that no ERK method has $r_{\mathcal{F}} > 0$ and is greater than fourth-order accurate. Maximum norm contractivity is closely related to positivity.[39] Positivity is particularly appealing because it ensures that physical quantities such as temperature and species concentrations remain forever nonnegative. The radius of positivity is the same as the radius of maximum norm contractivity.

To determine $r_{\mathcal{F}_2}$ we first define the matrices[16] $M_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j$, $B_{ij} = \text{diag}\{b_1, b_2, \dots, b_s\}$, and $\mathcal{M}_{il} = B_{ij}^{-1/2} M_{jk} B_{kl}^{-1/2}$. If $b_i > 0$, then $r_{\mathcal{F}_2} = -\frac{1}{\lambda_{\min}^{\mathcal{M}}}$ where $\lambda_{\min}^{\mathcal{M}}$ is the smallest eigenvalue of the matrix \mathcal{M}_{il} . A nonvanishing value of $r_{\mathcal{F}_\infty}$ requires that $b_i > 0$, $a_{ij} \geq 0$, and the Runge-Kutta K-function, $K(Z) = \det[I - (A - e b^T)Z]$, is absolutely monotonic on $[-r_{\mathcal{F}_\infty}, 0]$ where $Z = \{z_1, z_2, \dots, z_s\}$. $K(Z)$ is said to be absolutely monotonic at a point ξ if[52]

$$(2.22) \quad \frac{\partial^{i_1+i_2+\dots+i_s} K(\xi, \xi, \dots, \xi)}{\partial z_1^{i_1} \partial z_2^{i_2} \dots \partial z_s^{i_s}} \geq 0.$$

In the case of ERKs, each i_j may be equal to either 0 or 1. The largest magnitude of ξ on the negative real - axis for which these 2^s inequalities hold is denoted $-r_{\mathcal{F}_\infty}$. Alternatively for ERKs, one may enforce nonnegativity of

$$(2.23) \quad R(\xi), \quad \mathcal{A}(\xi) = \mathbf{A}(\mathbf{I} - \xi \mathbf{A})^{-1}, \quad \mathcal{B}(\xi) = \mathbf{b}^T(\mathbf{I} - \xi \mathbf{A})^{-1}, \quad \mathcal{E}(\xi) = (\mathbf{I} - \xi \mathbf{A})^{-1} \mathbf{e},$$

at $\xi = -r_{\mathcal{F}_\infty}$ where $\mathbf{e} = \{1, 1, \dots, 1\}$, $\mathbf{b} = b_i$, and $\mathbf{A} = a_{ij}$. Assuming that $b_i > 0$, $a_{ij} \geq 0$, these present 1, $(s-2)(s-1)/2$, $(s-1)$, and $(s-1)$ inequalities, respectively, or $s(s+1)/2$ in total. It should be noted that the region of circular contractivity is a circle located at $z = -r$ with radius $r_{\mathcal{F}_\infty}$ or $r_{\mathcal{F}_2}$, whichever is appropriate. This implies the property is likely most useful for parabolic rather than hyperbolic equations. For comparison purposes we follow Dahlquist and Jeltsch and write $r_{\mathcal{L}_2} = r_s$, the corresponding radius of the linear problem in an inner product norm,[57] i.e., the largest circle centered on the negative real - axis, fully contained in the left half-plane, that fits within the region where $|R(z)| = 1$. The linear analog of $r_{\mathcal{F}_\infty}$ is $r_{\mathcal{L}_\infty}$. The stability function, $R(Z)$, is said to be absolutely monotonic at a point ξ if[53] $\partial^i R(\xi)/\partial z^i \geq 0$, $i = 0, 1, 2, \dots, s$. The largest magnitude of ξ on the negative real - axis for which all of these $s+1$ inequalities hold is denoted $-r_{\mathcal{L}_\infty}$. Kraaijevanger[51] gives the maximum achievable $r_{\mathcal{L}_\infty}$ per stage for an m -stage method with order p , his optimal scaled threshold factors. We do not consider the internal stability of ERKs.[42, 43] Nonlinear instability caused by spurious triad wave interactions[79] in the spatial domain is outside the scope of this paper, but is probably best dealt with by using high-order filtering.[48]

2.6. Efficiency. Efficiency of a given s -stage ERK scheme may be considered from two decidedly different perspectives. One philosophy assumes that temporal integration error is acceptable and seeks to time step as briskly as possible. Simulations running on expensive supercomputers for hundreds of hours are under great pressure to be integrated as quickly as possible. Alternatively, integration may be conducted at some chosen maximum acceptable error. Virtually all DNS efforts that these authors are aware of implicitly subscribe to the former philosophy, due to computer resource limitations.

Stability-limited time stepping is the more primitive approach and only seeks to compare the relative efficiency of two schemes by using[69]

$$(2.24) \quad \eta^{(\text{stab})} = \frac{\lambda_1}{s_1} \left(\frac{\lambda_2}{s_2} \right)^{-1} = \frac{(\Delta t)_1 s_2}{(\Delta t)_2 s_1},$$

where λ is understood to be either the inviscid or viscous CFL number and scheme 1 is most efficient for $\eta^{(\text{stab})} > 1$. This term compares the distance integrated per unit of work (evaluations of $F(t, U(t)) = \text{number of stages}$) with no regard for the accuracy of integration and may be used to compare methods with arbitrary orders of accuracy and numbers of stages. For viscously or reactively dominated problems this term could be amended by replacing the CFL numbers with the respective $r_{\mathcal{F}_2}$ or $r_{\mathcal{F}_\infty}$ of each scheme.

Relative efficiencies of two q^{th} -order schemes based on an error limited time stepping procedure might best be measured by [40, 69]

$$(2.25) \quad \eta^{(\text{acc})} = \frac{s_2}{s_1} \left(\frac{A_2^{(q+1)}}{A_1^{(q+1)}} \right)^{\frac{1}{q+1}} = \frac{(\Delta t)_1^* s_2}{(\Delta t)_2^* s_1},$$

where scheme 1 is most efficient for $\eta^{(\text{acc})} > 1$. Slightly different from $\eta^{(\text{stab})}$, $\eta^{(\text{acc})}$ compares the distance integrated per unit of work at fixed integration error, $(\Delta t)^*$. We will consider the number of stages in a FSAL method as the effective number of stages for efficiency purposes. Obviously, for sufficiently large error tolerances, large time steps might exceed the linear stability bounds. In comparing schemes with different orders of accuracy we cannot use this last metric and simply paraphrase Shampine [69]. For sufficiently small error tolerances the higher order method is more efficient, but this argument does not imply that the lower order method is more efficient for large error tolerances. Prince and Dormand [62] note that only on the linear problem are lower order formulae sometimes preferable to higher order formulae. Sharp [71] finds that the higher-order methods are generally more accuracy efficient on nonstiff equations.

The choice of which efficiency measure should be used depends most strongly on what level of error is acceptable to the user. This, in turn, depends on what physical phenomena are being sought through the calculation. If integration at the linear stability limits produces sufficiently small error then, efficiency is best considered by using $\eta^{(\text{stab})}$; otherwise $\eta^{(\text{acc})}$ seems more appropriate. Spatial accuracy, another important matter that we do not consider here, must also be addressed. Strict temporal error tolerances make little sense without correspondingly strict spatial error tolerances. A future study on the spatial and temporal accuracy/resolution requirements associated with particular physical phenomena would be of tremendous utility to compressible DNS practitioners.

2.7. Simplifying Assumptions. Finally, in the course of designing several of the schemes in this paper, resorting to Butcher [8, 36] simplifying assumptions will be useful. On occasion, assumptions

$$(2.26) \quad C(\eta) : \quad \sum_{j=1}^s a_{ij} c_j^{q-1} = \frac{c_i^q}{q}, \quad i = 1, \dots, s, \quad q = 1, \dots, \eta,$$

$$(2.27) \quad D(\zeta) : \quad \sum_{i=1}^s b_i c_i^{q-1} a_{ij} = \frac{b_j}{q} (1 - c_j^q), \quad j = 1, \dots, s, \quad q = 1, \dots, \zeta,$$

will be invoked.

3. Two-Register Schemes. An s -stage ERK method placed in two-register vdH format (see van der Houwen[42], equation 2.2.4') takes on the Butcher array form

$$\begin{array}{c|ccccccc}
 0 & & & & & & & \\
 c_2 & a_{21} & & & & & & \\
 c_3 & b_1 & a_{32} & & & & & \\
 \vdots & \vdots & b_2 & a_{43} & & & & \\
 & & \vdots & b_3 & a_{54} & & & \\
 & & & \vdots & \ddots & \ddots & & \\
 c_s & & & & & b_{s-2} & a_{s,s-1} & \\
 \hline
 & b_1 & b_2 & b_3 & \cdots & b_{s-2} & b_{s-1} & b_s
 \end{array}$$

and allows $(2s - 1)$ degrees of freedom (DOF) to satisfy all constraints. In general, for an r -register method, there will be $r * s - r * (r - 1)/2$ DOF available. Conversely, $(s - r + 1) * (s - r)/2$ DOF are sacrificed for low storage. Setting $r = s$, the basic ERK method is retrieved with $s * (s + 1)/2$ DOF.

3.1. Two-Stage, Second-Order: RK2(2)[2R]. All two-stage, second-order ERKs may be used in 2R format. Minimum $A^{(3)} = 1/6$ occurs at $c_2 = a_{21} = 2/3$, $b_1 = 1/4$, $b_2 = 3/4$ with $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (0.791, 0.500)$. The maximally L_∞ contractive second-order method is Huen's method:[54] $c_2 = a_{21} = 1$, $b_1 = 1/2$, $b_2 = 1/2$ where $r_{\mathcal{F}_2} = r_{\mathcal{F}_\infty} = 1$ and $A^{(3)} = \sqrt{2}/6$. These are of only academic interest to the compressible DNS community because when implemented with centered, finite-difference methods on the convection-diffusion equation, the methods are unconditionally unstable in the inviscid limit.

3.2. Three-Stage, Third-Order: RK3(2)3[2R+]. The general solution to the two-register, three-stage, third-order vdH scheme has a one-parameter family of solutions along with two specific cases. These are readily derived by following Lambert's[54] three cases. For the cases when $c_2 \neq 0, \frac{2}{3}$, or c_3 and when $c_3 \neq 0$, the one parameter, c_3 , family of solutions is obtained for

$$(3.1) \quad c_2 = \frac{4 - 7c_3 + 6c_3^2 \pm \sqrt{c_3^2(17 - 60c_3 + 84c_3^2 - 48c_3^3)}}{6(1 - 2c_3 + 2c_3^2)},$$

provided c_2 is not complex. From this, Wray[90] suggests $c_3 = 2/3$, yielding $c_2 = 8/15$. Minimum principal error norm for the RK3(2)3[2R+]M is found by solving $\partial A^{(4)}/\partial c_3 = 0$ for c_3 by using the minus solution above. The result is that the minima occurs at $c_3 \approx \frac{81214816}{120777641}$ where $A^{(4)} = 0.04412$ and $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (0.521, 0.150)$. Maximum $r_{\mathcal{F}_\infty}$ occurs with RK3(2)3[2R+]N at $c_3 \approx \frac{23833}{37703}$ by using the plus solution where $A^{(4)} = 0.05094$ and $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (1.127, 0.838)$. Asking for contractivity of the embedded methods had the unfortunate consequence of increasing $E^{(4)}$ above optimal. The minimum principal error norm achievable for any explicit RK3()3 is $A^{(4)} = 0.041809$. Maximum radius of contractivity for the general RK3()3 is $r_{\mathcal{F}_\infty} = 1$ or $r_{\mathcal{F}_2} \approx 1.215$. All RK3()3 methods have $r_{\mathcal{L}_\infty} = 1$ and $r_{\mathcal{L}_2} = 1.256$.

In the two specific cases where $c_2 = c_3 = 2/3$ and $b_3 = 3/5$, then $A^{(4)} = 0.04630$ and $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (1.0, 0.6)$, and where $c_2 = 2/3$, $c_3 = 0$, $b_3 = (1 \mp \sqrt{17})/8$, both solutions have $A^{(4)} = 0.1326$ and are noncontractive. The former confluent solution admits only a defective embedded method. Stability limits of all three-stage, third-order, ERK schemes are $(\lambda, \lambda_v) = (0.87, 0.63)$ when integrating the convection-diffusion equation discretized with a sixth-order, tridiagonal, first-derivative operator.

3.3. Four-Stage, Third-Order: RK3(2)4[2R+]. Using two-registers over four stages allots degrees of freedom. Enforcing third-order accuracy, $\tau^{(k)} = 0, k = 1, 2, 3$, leaves three remaining DOF. For accuracy efficiency, RK3(2)4[2R+]C minimizes $A^{(4)}$ subject to $\Phi_4^{(4)} = 1/24$ in order to maximize linear stability and dissipation order. The resulting scheme is 6% more accuracy efficient than RK3(2)3[2R+]M, and has

$(\lambda, \lambda_v) = (1.42, 0.70)$; this scheme is listed in Tables 1 and 4 and shown in Figure 3.1. For nonlinear stability, RK3(2)4[2R+]CN seeks maximal $r_{\mathcal{F}_\infty}$ while achieving sixth-order dispersion error, $\phi_5 = 0$, by setting $\Phi_4^{(4)} = 1/30$. Of the maximum possible $r_{\mathcal{F}_\infty} = 2$ for any RK3()4[52] with $A^{(4)} = 0.03608$, RK3(2)4[2R+]CN achieves $r_{\mathcal{F}_\infty} = 1.007$ while keeping $A^{(4)} = 0.02870$. As with the RK3(2)3[2R+]N, a contractive embedded method drove $E^{(4)}$ to slightly greater than 1. If $\Phi_4^{(4)} = 1/48$, giving $(\lambda, \lambda_v) = (1.08, 1.30)$, $r_{\mathcal{L}_\infty} = 2$ is possible for RK3()4 methods.

3.4. Five-Stage, Fourth-Order: RK4(3)5[2R+]. Adding a fifth stage to a 2R-vdH scheme provides nine degrees of freedom. Fourth-order accuracy may now be considered. Eight order-of-accuracy constraints, $\tau^{(k)} = 0, k = 1, 2, 3, 4$, leave one DOF to optimize linear stability while maintaining acceptable accuracy via variation of $\Phi_9^{(5)}$. Tables 1 and 5 and Figure 3.1 give the $\Phi_9^{(5)} = 1/206$ solution, RK4(3)5[2R+]C, with $A^{(5)} = 0.005121$ and $(\lambda, \lambda_v) = (1.67, 1.21)$. Mated to this is an embedded scheme with $\Phi_4^{(4)} = 1/28$. We were unable to find any contractive methods for the RK4(3)5[2R+] or phase-lag methods having reasonable principal error norms. Setting $\Phi_9^{(5)} = 1/240$ gives $(\lambda, \lambda_v) = (1.62, 1.48)$ and the largest $r_{\mathcal{L}_\infty}$ for the RK4()5 methods is 2.

3.5. Six-Stage, Fourth-Order: RK4(3)6[2R+]. As additional stages can sometimes make for more efficient methods,[72] one may consider an RK4(3)6[2R+] scheme with three residual DOF after satisfying $\tau^{(k)} = 0, k = 1, 2, 3, 4$. Searching for solutions uncovered RK4(3)6[2R+]C with $A^{(5)} = 0.002148$ and $(\lambda, \lambda_v) = (1.97, 1.18)$. Unfortunately both $\eta^{(\text{acc})}$ and $\eta^{(\text{stab})}$ are less than those of RK4(3)5[2R+]C. No attempt was made to find a contractive solution. At $\Phi_9^{(5)} \approx 1/159$ and $\Phi_{20}^{(6)} \approx 1/2529$ where $(\lambda, \lambda_v) = (1.85, 1.62)$, $r_{\mathcal{L}_\infty}$ may reach ≈ 2.651 . For increased phase-lag accuracy one may set $\phi_5 = \phi_7 = 0$ to find $(\lambda, \lambda_v) = (0.29, 0.96)$ or may set $\phi_5 = \alpha_6 = 0$ to find $(\lambda, \lambda_v) = (0.35, 0.89)$. Minimizing dissipation error with $\alpha_6 = \alpha_8 = 0$ results in $\Phi_9^{(5)} = 1/128$, $\Phi_{20}^{(6)} = 1/1152$, and $(\lambda, \lambda_v) = (1.94, 1.09)$. With $A^{(5)} = 0.002509$, RK4(3)6[2R+]P{4,9} is such a scheme. Both RK4(3)6[2R+]C and RK4(3)6[2R+]P{4,9} use an embedded method with $\hat{\Phi}_4^{(4)} = 1/26$ and $\hat{\Phi}_9^{(5)} = 1/150$.

3.6. Nine-Stage, Fifth-Order: RK5(4)9[2R+]. A fifth-order, 2R-vdH scheme may be obtained in nine stages by solving the 17 unsimplified equations of condition, $\tau^{(k)} = 0, k = 1, 2, \dots, 5$, for the 17 free Butcher coefficients. Solution properties cannot be optimized. Over 800 distinct real roots to this system of equations have been found. The most accurate root found, RK5(4)9[2R+]M, has $A^{(6)} = 0.0006172$, but $(\lambda, \lambda_v) = (0.21, 1.03)$. The most stable method, RK5(4)9[2R+]S, has $A^{(6)} = 0.001014$, $(\lambda, \lambda_v) = (1.78, 1.59)$, and $(\hat{\lambda}, \hat{\lambda}_v) = (1.60, 1.61)$. A compromise solution, RK5(4)9[2R+]C, was found with $A^{(6)} = 0.0008209$, $(\lambda, \lambda_v) = (1.05, 1.29)$, and $(\hat{\lambda}, \hat{\lambda}_v) = (1.63, 1.15)$. An embedded method was designed for the three schemes by satisfying all eight fourth-order constraints plus setting $\hat{\Phi}_9^{(5)} = 1/135$. These methods are presented in Tables 1 and 6. Stability diagrams are provided in Figure 3.1. The largest linear positivity radius for these RK5(4)9 methods appears to be $r_{\mathcal{L}_\infty} \approx 4.095$ occurring at $\Phi_{20}^{(6)} \approx 1/779$, $\Phi_{48}^{(7)} \approx 1/7444$, $\Phi_{115}^{(8)} \approx 1/121935$, $\Phi_{286}^{(9)} \approx 1/4494000$, where $(\lambda, \lambda_v) = (0.34, 2.24)$.

4. Three-Register Schemes. Applications having slightly less stringent memory constraints may add an additional storage register per ODE. Extending the vdH methodology to three-registers, an s -stage scheme

takes the Butcher array form

$$\begin{array}{c|cccccc}
0 & & & & & & \\
c_2 & a_{21} & & & & & \\
c_3 & a_{31} & a_{32} & & & & \\
\vdots & b_1 & a_{42} & a_{43} & & & \\
& \vdots & b_2 & a_{53} & a_{54} & & \\
& & \vdots & \ddots & \ddots & \ddots & \\
c_s & & & & b_{s-3} & a_{s,s-2} & a_{s,s-1} \\
\hline
& b_1 & b_2 & \cdots & b_{s-3} & b_{s-2} & b_{s-1} & b_s
\end{array}$$

where there are now $(3s - 3)$ independent coefficients that may be used to satisfy particular conditions. Alternatively, $(s - 2) * (s - 3)/2$ coefficients are lost to low storage.

4.1. Three-Stage, Third-Order: RK3(3)[3R]. Any three-stage, third-order ERK method may be implemented in 3R format. As such, one may seek the method having the smallest principal error norm. By setting $\partial A^{(4)}/\partial c_2 = 0$ and $\partial A^{(4)}/\partial c_3 = 0$ from the two-parameter family of solutions it is found that $c_2 \approx \frac{73459324}{147952825}$, $c_3 \approx \frac{245463752}{326524211}$, $A^{(4)} = 0.041809$, and $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (0.894, 0.0)$. The relation of c_2 and c_3 to the various other Butcher coefficients may be found in the literature.[9, 21, 35, 54] Stability limits are identical to the RK3(2)3[2R+] methods. Maximal contractivity, $r_{\mathcal{F}_\infty} = r_{\mathcal{F}_2} = 1$, is found in Fehlberg's[26, 52, 74] method with $c_2 = 1$, $c_3 = 1/2$, and $A^{(4)} = 0.07217$, while for Cooper's scheme[15] in an inner product norm where $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (1.215, 0.691)$, $c_2 \approx 270/251$, $c_3 \approx 166/305$, and $A^{(4)} = 0.07221$.

4.2. Four-Stage, Third-Order: RK3(2)4[3R+]. Kraaijevanger[52] has shown that optimizing the radius of maximum norm contractivity for general third-order ERKs allows one to obtain $r_{\mathcal{F}_\infty} = (s - 2)$ for $s = 3, 4$. For $s \geq 5$, $r_{\mathcal{F}_\infty} \leq (s - \sqrt{s})$. A family of third-order schemes given by four unique Butcher coefficients, $b_i = (s - 2)/(s(s - 1))$, $i = 1, 2, \dots, (s - 1)$, $b_s = 2/s$, $a_{ij} = 1/(s - 2)$, $i = 2, 3, \dots, (s - 1) > j$, $a_{sj} = 1/(2(s - 1))$, $j = 1, 2, \dots, (s - 1)$, which for $s = 3, 4$ constitute the maximally L_∞ contractive methods. From these relations it is seen that $c_{s-1} = 1$ and $c_s = 1/2$. For $s = 5, 6, 7$, and 8 one finds for this family that $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty})$ is given by $(2.449, 2.202)$, $(2.828, 2.347)$, $(3.162, 2.460)$, and $(3.464, 2.553)$. For reduced storage we set $b_1 = (s - 2)/(s(s - 1)) = a_{s1} = 1/(2(s - 1))$ to find $s = 4$. The resulting method, RK3(2)4[3R+]N, is essentially given by Kraaijevanger with $r_{\mathcal{F}_\infty} = r_{\mathcal{F}_2} = r_{\mathcal{L}_\infty} = r_{\mathcal{L}_2} = 2$ and $A^{(4)} = 0.03608$. A good embedded method for this scheme is $\hat{b}_i = \{8, 9, 8, 60\}/85$.

4.3. Four-Stage, Fourth-Order: RK4(4)[3R]. From the general solution to the four-stage, fourth-order ERK scheme,[9, 21, 35] it is found that there is a one-parameter family of 3R solutions and three specific solutions. The one-parameter family of solutions is given by

$$(4.1) \quad c_3 = \frac{(20 - 50c_2 + 36c_2^2) \pm \sqrt{(-20 + 50c_2 - 36c_2^2)^2 - 4(9 - 26c_2 + 16c_2^2)(16 - 36c_2 + 36c_2^2)}}{2(16 - 36c_2 + 36c_2^2)},$$

where $0, c_2, c_3, 1$ are all distinct, $c_2 \neq 1/2$, $3 - 4(c_2 - c_3) + 6c_2c_3 \neq 0$, and c_3 is not complex. The principal error norm is minimized by setting $\partial A^{(5)}/\partial c_2 = 0$ where RK4(4)[3R]M is found for the plus solution with $c_2 \approx \frac{79947400}{181010101}$, $r_{\mathcal{F}_2} = 0.718$, and $A^{(5)} = 0.01263$. Maximal $r_{\mathcal{F}_2} = 0.882$ occurs with the plus solution RK4(4)[3R]N at $c_2 \approx \frac{1612}{3517}$ (with $A^{(5)} = 0.01319$) for 3R methods and $r_{\mathcal{F}_2} = 1.144$ for Cooper's[15] RK4(4) method. These values compare with $r_{\mathcal{F}_2} = 1$ and $A^{(5)} = 0.01450$ for the "classical Runge-Kutta" (see Butcher[9], §313) and $A^{(5)} = 0.011977$ for the absolute minimum principal error norm for any four-stage, fourth-order, ERK scheme. Kraaijevanger[52] has shown that there exists no L_∞ contractive RK4(4) method. Adding a third-order embedded scheme to this method is impossible unless FSAL techniques are used but

we do not pursue this matter. Instead of a FSAL pair, complete use of the fifth stage generally makes for more efficient schemes. One potential exception is inviscid stability efficiency ($\lambda/s \approx 0.355$). The three other specific cases are found using Butcher's cases 3, 4, and 5 in §312.[9] In case 3, $b_3 = -2/15$ and $A^{(5)} = 0.03416$, in case 4, $b_4 = 3/10$ and $A^{(5)} = 0.02330$, while in case 5, $c_2 = 3/7$ and $A^{(5)} = 0.01282$. None of these last three schemes is contractive. Linear stability limits on the convection-diffusion equation for the RK4()4[3R] are $(\lambda, \lambda_v) = (1.42, 0.70)$, $r_{\mathcal{L}_\infty} = 1$, and $r_{\mathcal{L}_2} = 1.393$.

4.4. Five-Stage, Fourth-Order: RK4(3)5[3R+]. Three additional degrees of freedom afforded by adding a third register to the RK4(3)5[2R+] method may be put to good use. Optimizing accuracy, RK4(3)5[3R+]M has $A^{(5)} = 0.001884$ and $(\lambda, \lambda_v) = (0.22, 0.81)$ where $\tau_{3,9}^{(5)} = 0$. A similar method of Prince has $\tau_{4,6,8,9}^{(5)} = 0$. A balance between linear stability and low error is found in RK4(3)5[3R+]C with $A^{(5)} = 0.003859$ and $(\lambda, \lambda_v) = (1.67, 1.17)$. It should be noted that for the RK4(3)5[3R+]C, selection of $\Phi_9^{(5)} = 1/200$ forces $A^{(5)} \geq 0.003333$, as can be seen from $A_\infty^{(5)}$. Contractivity appears to be maximized with RK4(3)5[3R+]N having $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (0.995, 0.477)$, $A^{(5)} = 0.004587$, and $(\lambda, \lambda_v) = (1.67, 1.20)$. Although not nearly as contractive as Kraaijevanger's RK4()5 scheme, it has 7% better $\eta^{(\text{acc})}$. Each of these three schemes is presented in Tables 2 and 5. Stability plots are given in Figure 4.1. Two highly accurate RK4(3)5[3R+]P{4,7} schemes where $\Phi_9^{(5)} = 1/144$ and $(\lambda, \lambda_v) = (1.74, 0.89)$ were found with $A^{(5)} = 0.002658$ and $A^{(5)} = 0.002857$, but neither would accept an embedded method with a reasonably large linear stability region.

4.5. Six-Stage, Fifth-Order: RK5()6[3R]. With only 15 degrees of freedom simplifying assumption $D(1)$ may be invoked to reduce the number of condition equations from 17 to 15. By doing so, a fourth-order embedded scheme is no longer possible. At least 13 schemes like this exist; the most accurate found, RK5()6[3R]M, has $A^{(6)} = 0.003678$ with $(\lambda, \lambda_v) = (0.20, 0.72)$.

4.6. Seven-Stage, Fifth-Order: RK5(4)7[3R+]. To get a 5(4) pair, a seventh stage is added and only simplifying assumption $C(2)$ is utilized. This results in 18 equations in 18 unknowns for the main scheme and 7 equations in 7 unknowns for the embedded method. Of the 7 schemes found, the best one is RK5(4)7[3R+]M with $A^{(6)} = 0.002213$, $(\lambda, \lambda_v) = (0.28, 0.92)$, $(\hat{\lambda}, \hat{\lambda}_v) = (0.95, 0.59)$, and $B^{(6)} < 1.0$. Adding an extra stage to this method, however, can lead to a method with as much as 38% better $\eta^{(\text{acc})}$, as will be shown in section 4.7. Maximum $r_{\mathcal{L}_\infty} \approx 2.654$ occurs at $\Phi_{20}^{(6)} \approx 1/955$, $\Phi_{48}^{(7)} \approx 1/17733$ with $(\lambda, \lambda_v) = (0.28, 1.60)$.

4.7. Eight-Stage, Fifth-Order -RK5(4)8[3R+]. An eight-stage, three-register vdH scheme has 21 degrees of freedom. Seeking a 5(4) pair, Butcher simplifying assumption $C(2)$ is applied. The resulting system of equations necessary to satisfy all order conditions is

$$(4.2) \quad \begin{aligned} \tau_1^{(k)} &= 0, \quad k = 1, 2, \dots, 5, \quad \sum_{j=1}^s a_{ij}c_j = c_i^2/2, \quad i = 3, 4, \dots, 8, \\ \tau_3^{(4)} &= \tau_{4,5,8}^{(5)} = b_2 = \sum_{i=3}^s b_i a_{i2} = \sum_{i=3}^s b_i c_i a_{i2} = \sum_{i,j=3}^s b_i a_{ij} a_{j2} = 0, \end{aligned}$$

for the main scheme and

$$(4.3) \quad \hat{\tau}_1^{(k)} = 0, \quad k = 1, 2, 3, 4, \quad \hat{b}_2 = \hat{\tau}_3^{(4)} = \sum_{i=3}^s \hat{b}_i a_{i2} = 0,$$

for the embedded scheme. Optimization may now be done with two remaining DOF in the main method and one in the embedded method. A numerical search found two low-error solution families (among 25 or so), the first with more desirable stability properties and the second having lower $A^{(6)}$. RK5(4)8[3R+]C,

RK5(4)8[3R+]P{8,7}, and RK5(4)8[3R+]M are given in Tables 2 and 6. The first two come from the more stable family. RK5(4)8[3R+]C has $A^{(6)} = 0.0008306$ with $(\lambda, \lambda_v) = (1.30, 1.52)$ while RK5(4)8[3R+]P{8,7} has $A^{(6)} = 0.0007923$ with $(\lambda, \lambda_v) = (1.01, 1.20)$. RK5(4)8[3R+]M achieves $A^{(6)} = 0.0003240$, but $(\lambda, \lambda_v) = (0.32, 1.00)$. The final degree of freedom for the embedded methods is used to set $\tilde{\Phi}_9^{(5)} = 1/130, 1/135, 1/122.5$ in the RK5(4)8[3R+]C, P, M schemes, respectively. Stability plots for the three schemes are shown in Figure 4.1.

Enhanced dispersion/dissipation order is enforced with

$$(4.4) \quad \begin{aligned} \Phi_{20}^{(6)} &= (1 + 2268\Phi_{115}^{(8)})/756 & \Phi_{48}^{(7)} &= (1 + 22680\Phi_{115}^{(8)})/7560 & (\phi_7 = \phi_9 = 0), \\ \Phi_{20}^{(6)} &= 1/720 & \Phi_{48}^{(7)} &= (1 + 5760\Phi_{115}^{(8)})/5760 & (\alpha_6 = \alpha_8 = 0), \\ \Phi_{20}^{(6)} &= 1/720 & \Phi_{48}^{(7)} &= 1/5040 & (\alpha_6 = \phi_7 = 0). \end{aligned}$$

With the RK5(4)8[3R+]M solution family, the methods RK5(4)8[3R+]PM{10,5}, RK5(4)8[3R+]PM{8,7}, and RK5(4)8[3R+]PM{6,9} may be found having $A^{(6)} = 0.0005049, 0.0005946$, and 0.0005525 , and $(\lambda, \lambda_v) = (0.35, 1.14), (0.88, 0.98)$, and $(0.53, 1.04)$, respectively. Each may be fitted with a high-quality embedded method by setting $\tilde{\Phi}_9^{(5)} = 1/130$. In each of these methods, $D < 2$, $B^{(6)}, C^{(6)} < 1.5$ and $E^{(6)} < 0.5$. The largest possible $r_{\mathcal{L}_\infty}$ for RK5(4)8 schemes is found at $\Phi_{20}^{(6)} \approx 1/834$, $\Phi_{48}^{(7)} \approx 1/9862$, $\Phi_{115}^{(8)} \approx 1/266413$ where $r_{\mathcal{L}_\infty} \approx 3.368$ and $(\lambda, \lambda_v) = (0.30, 1.89)$.

5. Four-Register Schemes. Further relaxing the memory constraints, the 4R-vdH scheme structure appears as

$$\begin{array}{c|cccccccc} 0 & & & & & & & & \\ c_2 & a_{21} & & & & & & & \\ c_3 & a_{31} & a_{32} & & & & & & \\ c_4 & a_{41} & a_{42} & a_{43} & & & & & \\ \vdots & b_1 & a_{52} & a_{53} & a_{54} & & & & \\ & \vdots & b_2 & a_{63} & a_{64} & a_{65} & & & \\ & & \vdots & \ddots & \ddots & \ddots & \ddots & & \\ c_s & & & & b_{s-4} & a_{s,s-3} & a_{s,s-2} & a_{s,s-1} & \\ \hline & b_1 & b_2 & \cdots & b_{s-4} & b_{s-3} & b_{s-2} & b_{s-1} & b_s \end{array}$$

and has $(4s - 6)$ DOF. Storage reduction has consumed $(s - 3) * (s - 4)/2$ of them.

5.1. Four-Stage, Fourth-Order: RK4(4)[4R]. In cases where the number of stages equals the number of available storage registers, all possible schemes may be implemented in sR-vdH fashion. For the four-stage, fourth-order ERK, we solve for the minimum error scheme. Setting $\partial A^{(5)}/\partial c_2 = 0$ and $\partial A^{(5)}/\partial c_3 = 0$, results in $c_2 \approx \frac{63753230}{178211381}$, $c_3 \approx \frac{131894393}{222986851}$, $A^{(5)} = 0.0119775$, and $r_{\mathcal{F}_2} = 0.613$. The relation between the various other Butcher coefficients may be found in the literature.[9, 21, 35] Stability limits are $(\lambda, \lambda_v) = (1.42, 0.70)$. Again, a third-order embedded method is impossible with this scheme without FSAL constructs. Maximal inner product norm contractivity occurs with Cooper's RK4(4) scheme at $c_2 \approx \frac{7723}{13798}$ and $c_3 \approx \frac{6075}{13798}$ where $r_{\mathcal{F}_2} = 1.14373$ and $A^{(5)} = 0.01755$. Gottlieb and Shu[31] use Butcher's[9] case 2 in §312, setting $b_3 = \frac{7873}{30000}$ to get $A^{(5)} = 0.01592$ and $r_{\mathcal{F}_2} = 0.945$. In all RK4(4) cases $r_{\mathcal{F}_\infty} = 0$, $r_{\mathcal{L}_\infty} = 1$, and $r_{\mathcal{L}_2} = 1.393$.

5.2. Five-Stage, Fourth-Order: RK4(3)5[4R+]. An RK4(3)5[4R+] method has 14 DOF, having sacrificed only 1 DOF to low storage. To minimize $A^{(5)}$, Butcher simplifying assumptions $C(2)$ and $D(1)$ are applied, reducing the constraint system to

$$(5.1) \quad \begin{aligned} \tau_1^{(k)} &= 0, \quad k = 1, 2, 3, 4, \quad c_5 = 1, \quad \tau_4^{(5)} = \varepsilon, \quad b_2 = \sum_{i=3}^s b_i c_i a_{i2} = 0, \\ \sum_{j=1}^s a_{ij} c_j &= c_i^2/2, \quad i = 3, 4, \quad \sum_{i=1}^s b_i a_{ij} = b_j(1 - c_j), \quad i = 2, 3, 4. \end{aligned}$$

An exact one-parameter, c_4 , solution has been found where $A^{(5)}$ may be made arbitrarily small. For $\varepsilon = 0$, $A^{(5)} = \sqrt{103/1036800}(c_4 - 1)$. Unfortunately, both b_4 and b_5 are proportional to $(c_4 - 1)^{-1}$, a so-called limiting formula. As $c_4 \rightarrow 1$, $D = b_4 = -[12(c_4 - 1)c_4(5c_4 - 2)]^{-1}$. Setting $\varepsilon = -1/40000$ and $c_4 = 199/200$, RK4(3)5[4R+]M has $A^{(5)} = 0.00003216$, $A^{(6)}/A^{(5)} = 130.3$, and $D = 6.365$.

To obtain a contractive RK4(3)5[4R+] scheme, we closely follow Kraaijevanger[52] with the exception of not enforcing $(a_{51} - r_{\mathcal{F}_\infty} a_{54} a_{41})$. Note that we solved 15 equations (8 order conditions and 7 of his 8 contractivity conditions) in 15 unknowns whereas Kraaijevanger performed an optimization problem. Kraaijevanger's RK4()5 method has $A^{(5)} = 0.006439$, $(\lambda, \lambda_v) = (1.64, 1.34)$, and $(r_{\mathcal{L}_2}, r_{\mathcal{L}_\infty}, r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (2.191, 1.861, 1.835, 1.508)$. The RK4(3)5[4R+]N method has $A^{(5)} = 0.005635$, $(\lambda, \lambda_v) = (1.63, 1.40)$, and $(r_{\mathcal{F}_2}, r_{\mathcal{F}_\infty}) = (1.733, 1.095)$. We mention that a good embedded method may be added to Kraaijevanger's RK4()5 scheme by solving the four third-order embedded order conditions, linear in the \hat{b}_i 's, by setting $\hat{b}_5 = 113/599$. Coefficients and properties of the two RK4(3)5[4R+] methods are listed in Tables 3 and 5. Stability plots are given in Figure 5.1.

5.3. Six-Stage, Fifth-Order: RK5(4)6[4R+]. By increasing the stage count to six, a 5(4) pair may be considered with Butcher simplifying assumption $C(3)$. The general RK5(4)6[4R+] method has 18 DOF in the main scheme and 6 DOF in the embedded method. Of the nine main schemes found, the best scheme has $A^{(6)} = 0.001961$ and $(\lambda, \lambda_v) = (0.28, 0.99)$. A more ambitious agenda uses only simplifying assumption $C(2)$ while enforcing a condition on a_{i2} . To do this we solve

$$(5.2) \quad \begin{aligned} \tau_1^{(k)} &= 0, \quad k = 1, 2, \dots, 5, \quad \sum_{j=1}^s a_{ij} c_j = c_i^2/2, \quad i = 3, 4, 5, 6, \quad \tau_3^{(4)} = \tau_{4,5,8}^{(5)} = 0, \\ b_2 &= \sum_{i=3}^s b_i a_{i2} = \sum_{i=3}^s b_i c_i a_{i2} = \sum_{i,j=3}^s b_i a_{ij} a_{j2} = 0, \quad a_{42} = \frac{c_3(3c_4 - 12c_4^2 + 10c_4^3)}{2c_2(3 - 12c_3 + 10c_3^2)}, \end{aligned}$$

for the main scheme and

$$(5.3) \quad \hat{\tau}_1^{(k)} = 0, \quad k = 1, 2, 3, 4, \quad \hat{b}_2 = 0, \quad \Phi_9^{(5)} = 1/130.$$

for the embedded method. Note that the strategies described by Papakostas et al.[60] and Hairer et al.[35] (§II.5) must be modified slightly. Tables 3 and 6 show RK5(4)6[4R+]M having $A^{(6)} = 0.0009449$ and $(\lambda, \lambda_v) = (0.31, 0.93)$. A stability diagram for this scheme is given in Figure 5.1. With $\Phi_{20}^{(6)} = 1/1440$, $r_{\mathcal{L}_\infty}$ reaches 2 for the RK5(4)6 method. A FSAL method akin to those of Dormand et al.[19, 20] and Papakostas et al.[60] is not considered.

5.4. Seven-Stage, Fifth-Order - RK5(4)7[4R+]. A seven-stage, 5(4) pair may be approached in at least four ways: using $C(2)$, $C(3)$, $C(2)$ and $D(1)$, or $C(3)$ and $D(1)$. To satisfy all fifth-order constraints, these require 18, 20, 18, and 21 DOF, respectively. For sixth-order these increase to 30, 28, 24, and 25. In addition, use of $C(3)$ reduces the number of embedded order conditions. The simplest approach is to use $C(3)$ and $D(1)$. Setting $\tau_6^{(6)} \approx 2 \times 10^{-6}$, a solution was found having $A^{(6)} = 0.0003974$ and $(\lambda, \lambda_v) = (0.30, 0.87)$. With only $C(3)$, a somewhat better solution has $A^{(6)} = 0.0003649$ and $(\lambda, \lambda_v) = (0.32, 0.89)$.

To decrease $A^{(6)}$ further, only $C(2)$ is assumed. Using a FSAL method allows the main scheme to be designed independently of the embedded method. For fifth order in the main method,

$$(5.4) \quad \begin{aligned} \tau_1^{(k)} &= 0, \quad k = 1, 2, 3, 4, 5, \quad \tau_3^{(4)} = \tau_{4,5,8}^{(5)} = 0, \\ b_2 &= \sum_{i=3}^s b_i a_{i2} = \sum_{i=3}^s b_i c_i a_{i2} = \sum_{i,j=3}^s b_i a_{ij} a_{j2} = 0, \quad \sum_{j=1}^s a_{ij} c_j = c_i^2/2, \quad i = 3, 4, 5, 6, 7, \end{aligned}$$

and for the fourth-order embedded method,

$$(5.5) \quad \hat{\tau}_1^{(k)} = 0, \quad k = 1, 2, 3, 4, \quad \hat{b}_2 = \sum_{i=3}^s \hat{b}_i a_{i2} = \hat{\tau}_3^{(4)} = 0.$$

For phase-lag methods, which we do not pursue, select $(\phi_7 = \phi_9 = 0)$ by setting $\Phi_{20}^{(6)} = 1/756$ and $\Phi_{48}^{(7)} = 1/7560$ $[(\lambda, \lambda_v) = (0.36, 1.16)]$, $(\alpha_6 = \phi_7 = 0)$ by setting $\Phi_{20}^{(6)} = 1/720$ and $\Phi_{48}^{(7)} = 1/5040$ $[(\lambda, \lambda_v) = (0.88, 0.99)]$, or $(\alpha_6 = \alpha_8 = 0)$ by placing $\Phi_{20}^{(6)} = 1/720$ and $\Phi_{48}^{(7)} = 1/5760$ $[(\lambda, \lambda_v) = (0.53, 1.05)]$. Note that RK5(4)8[4R+]FM has $\alpha_6 \approx \phi_7 \approx 0$.

0									
c_2	a_{21}								
c_3	a_{31}	a_{32}							
c_4	a_{41}	a_{42}	a_{43}						
c_5	a_{51}	a_{52}	a_{53}	a_{54}					
\vdots	b_1	a_{62}	a_{63}	a_{64}	a_{65}				
\vdots	\vdots	b_2	a_{73}	a_{74}	a_{75}	a_{76}			
	\vdots	\ddots	\ddots	\ddots	\ddots	\ddots			
c_s			b_{s-5}	$a_{s,s-4}$	$a_{s,s-3}$	$a_{s,s-2}$	$a_{s,s-1}$		
	b_1	b_2	\cdots	b_{s-5}	b_{s-4}	b_{s-3}	b_{s-2}	b_{s-1}	b_s

6.1. Seven-Stage, Fifth-Order: RK5(4)7[5R+]. A seven-stage, five-register, 5(4) pair may be reached as if it were a 6(4) pair. Both pairs $C(2)$, $D(1)$ and $C(3)$, $D(1)$ enable a sixth-order main method that requires 24 and 25 DOF, respectively. We will follow the strategy of Sharp and Smart[72] and Macki and Shampine[6] by solving for the sixth-order method and then will pollute it ever so slightly. For sixth-order main method with $C(3)$ and $D(1)$ we enforce

and for the fourth-order embedded method,

Interestingly, in spite of the nonlinearity in the b_i 's, $b_7 = 1/12$. Setting $\tau_1^{(6)} = 2 \times 10^{-5}$, $\tau_6^{(6)} = \sum_{i=3}^s b_i c_i^2 a_{i2} = \sum_{i,j=3}^s b_i c_i a_{ij} a_{j2} = 5 \times 10^{-7}$, all 20 $\tau_i^{(6)}$ are nearly equally corrupted. The resulting method, RK5(4)7[5R+J]M, has $A^{(6)} = 0.000008959$, $A^{(7)} = 0.0005771$, $A^{(8)} = 0.0008997$, $A^{(9)} = 0.001007$, $A^{(7)}/A^{(6)} = 64.42$, $(\lambda, \lambda_v) = (0.92, 0.99)$, and $(\hat{\lambda}, \hat{\lambda}_v) = (1.05, 1.19)$. Tables 3 and 6 and Figure 6.1 display this scheme.

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we have chosen to contrast our third-order schemes to that of Sharp and Smart[73][SS-RK3(2)4], fourth-order schemes to that of Prince,[21][P-RK4(3)5], and fifth-order methods to those of Bogacki and Shampine,[6][BS-RK5(4)7], Sharp and Smart,[72][SS-RK5(4)7], Dormand and Prince,[19][DOPRI5-RK5(4)7FM], and Papakostas and Papageorgiou,[60][PP-RK5(4)7F]. These reference methods have been chosen because they appear to be the best available full-storage methods within their respective classes. The memory requirement of these full-storage methods is not less than the stage number for non-FSAL methods or the effective number of stages for FSAL methods.

All schemes presented in this paper have been designed, at a minimum, to avoid any obvious problems. As is usual in the design of ERK methods, great emphasis is placed on reducing $A^{(q+1)}$ to as low as possible. DETEST results are well correlated with this measure. DETEST runs involve 25 separate integrations (A1-E5) in 5 general categories (A-E). Error is computed by taking the geometric mean of the worst performances in each of the 5 categories by using the PI-controller. $A^{(q+2)}$ may sometimes be seen to affect scheme performance at lax tolerances. Embedded “quality” parameters $B^{(p+2)}$, $C^{(p+2)}$, and $E^{(p+2)}$ of the low-storage schemes are generally quite reasonable, and embedded linear stability domains are commensurate with their main methods. The largest Butcher coefficient, D , never exceeds 7 in any low-storage method and for most schemes is near unity. In addition, none of the low-storage methods have defective embedded methods.

Reduced-storage, third-order schemes appear to forfeit little relative to corresponding full-storage schemes. At 3 stages, linear stability is identical among all schemes. Accuracy-based efficiency may be brought to 99% of the maximum achievable with RK3(2)3[2R+]M. Nonlinear stability may be made equal to 84% of Fehlberg’s three-stage, third-order method with RK3(2)3[2R+]N while simultaneously requiring 9% less work for similar error tolerances. High quality embedded methods are easily added to these schemes. Adding a fourth stage to a 3(2) pair appears to lead to 6% higher $\eta^{(acc)}$ with RK3(2)4[2R+]C relative to RK3(2)3[2R+]M. Inviscid stability efficiency also jumps from $\lambda/s = 0.290$ to $\lambda/s = 0.355$. If accuracy or inviscid stability efficiency is a priority, this scheme is the best third-order method presented and behaves similarly to the 3(2) pair of Sharp and Smart [SS-RK3(2)4]. Efficiencies of these last two methods may be seen in Figure 7.1, a comparison of third- and fourth-order methods using DETEST, as well as in Table 4. Viscous stability efficiency and contractivity, however, favor the three-stage 3(2) pairs, $\lambda_v/s = 0.210$ versus $\lambda_v/s = 0.175$. RK3(2)3[2R+]N has $r_{\mathcal{F}_\infty}/s = 0.279$, compared to $r_{\mathcal{F}_\infty}/s = 0.252$ for RK3(2)4[2R+]CN, while also being 16% more accuracy efficient. Where contractivity is the primary concern, RK3(2)4[3R+]N nearly doubles the normalized contractivity radius of Fehlberg’s RK3(2)3 method ($r_{\mathcal{F}_\infty}/s = 0.333$), while still only using 3 registers. The price of achieving $r_{\mathcal{F}_\infty}/s = 0.500$ is relatively poor $\eta^{(acc)}$, 77% of SS-RK3(2)4.

A quick survey of existing third-order methods includes several reduced storage methods by Carpenter and Kennedy,[11, 12] Williamson[87], and Wray[90]. Neither the original Williamson nor Wray schemes has an embedded method; they have accuracy efficiencies within 0.1% of each other. Of the two methods given by Carpenter and Kennedy, both Williamson-type schemes, one is clearly the most accurate third-order scheme given in Table 4 but has no error control capabilities, an easily rectifiable matter, while the other sacrifices efficiency to achieve an embedded method with no storage penalty. Bogacki and Shampine[5] have clearly improved upon Fehlberg’s two 3(2), or 2(3), pairs but the method of Sharp and Smart appears to be the best full-storage 3(2) pair.

Comparing RK4(3)5[2R+]C with the third-order schemes, the fourth-order method is generally not only more stability efficient, but a DETEST comparison of all 2R+ methods, given in Figure 7.2, shows that it can achieve moderate error tolerances at a small fraction of the work needed by the lower order

methods. RK4(3)5[2R+]C seems the more prudent choice over any 3(2) pair for all tolerances below $\approx 10^{-1}$. Contractivity aside, RK4(3)5[2R+]C is quite a bargain.

Optimizing within fourth-order methods may take many directions, with RK4(3)5[2R+]C serving as a good reference. Figures 7.1 and 7.3 show DETEST results on the relative efficiencies of all fourth-order schemes and of all three register methods. Table 5 shows that adding a third register, in principle, allows for a 6% increase in efficiency with RK4(3)5[3R+]C. Using RK4(3)5[2R+]C or RK4(3)5[3R+]C enables $\lambda/s = 0.334$ and $\lambda_v/s \approx 0.238$. Where accuracy but not stability efficiencies are most important, RK4(3)5[3R+]M and RK4(3)5[4R+]M are 22% and 176% more efficient according to Table 5. It may be seen in Figure 7.1 that those numbers are not achieved until quite tight tolerances are reached. DETEST results of 4R+ methods, Figure 7.4, show that RK4(3)5[4R+]M is as efficient as RK5(4)6[4R+]M, whose $\eta^{(\text{acc})}$ is 62%, to tolerances of $\approx 10^{-8}$! RK4(3)5[4R+]M is acting like a fifth-order method having an $\eta^{(\text{acc})}$ of 58% as determined by comparing $A^{(6)}$. Both of these 4(3) “M” methods compare favorably with the best contemporary full-storage 4(3) pair of Prince.[21] Maximum norm contractivity of fourth-order methods, on a per stage basis, offers slightly less possibility than third-order methods. Kraaijevanger’s RK4()5 method is the most contractive RK4()5 with $r_{\mathcal{F}_\infty}/s = 0.302$, a bit less than Fehlberg’s $r_{\mathcal{F}_\infty}/s = 0.333$. This reduction is particularly noticeable when additional requirements like low-storage are imposed. With four registers, at least $r_{\mathcal{F}_\infty}/s = 0.219$ is possible, but this result is likely reduced to $r_{\mathcal{F}_\infty}/s = 0.095$ at three registers. These results, along with the fact that contractive ERKs do not exist at fifth order, suggest that there is a trade-off between contractivity and order of accuracy. This trade-off may not be so unfortunate because the linear positivity radius, $r_{\mathcal{L}_\infty}$, remains substantial for many high-order methods and it is likely that the perceived need for large $r_{\mathcal{F}_\infty}$ values is partially attributable to poor temporal error control. Gottlieb and Shu[31] compare two second-order methods and find that the noncontractive method, although it has 43.85 times the principal error norm of the contractive method performs less well. We inspect existing 4(3) pairs and avoid the methods of Fehlberg[26] and Merson[35] because they have defective embedded schemes when used in local extrapolation mode. Neither Zonneveld’s method[35] nor Nørsett’s method[22] are particularly efficient even with full storage. The former method may also have an unreliable error estimate on inviscid problems at lax tolerances. Even though Stanescu and Habashi[77] offer a 2N method, it lacks both error control and efficiency. In the event that overwriting of the U -vector is not possible, the RK4()5[2N]C method of Carpenter and Kennedy,[11] fitted with an embedded method, would be preferable to RK4(3)5[2R+]C because the 2N method is 4% more efficient. Compared to Prince’s RK4(3)5 method, RK4(3)5[3R+]M is largely the same yet uses only three registers, while RK4(3)5[4R+]M is substantially more efficient.

The burden of low storage becomes apparent relative to corresponding contemporary pairs at fifth order because of the large number of forsaken degrees of freedom as well as the large amount of research that has gone into optimizing existing 5(4) pairs. This burden may easily be seen in Figure 7.5, a DETEST comparison of fifth-order methods. Optimization of lower order methods would seem to have taken a back seat to those fifth order and higher for reasons of efficiency. In order to achieve fifth order in 2 registers and 9 stages, 28 DOF are sacrificed! Not surprisingly, $\eta^{(\text{acc})}$ of 41-45% relative to BS-RK5(4)7 is seen in Table 6. This relative inefficiency makes the RK5(4)9[2R+] methods clearly more efficient than the RK4(3)5[2R+]C only at tolerances of $\approx 10^{-5}$ to 10^{-6} , and DETEST shows both RK4(3)5[3R+]M and RK4(3)5[4R+]M to always be more efficient. To their defense, the RK5(4)9[2R+] methods have been derived with no residual DOF for optimization purposes, used no simplifying assumptions, and by virtue of the low-storage strategy, the order conditions became horribly nonlinear in the b_i ’s. The brighter side of the relatively high stage number is that stability efficiency can be quite high for 5(4) pairs. We hasten to add that if stability efficiency is desired

then RK4(3)5[2R+]C should be accurate enough while allowing for much larger time steps. Accepting a third register in a fifth-order method allows for accuracy efficiencies to move from 41-45% of BS-RK5(4)7 to 48-56%, while stability efficiencies stay the same or decline. For acoustic applications, RK5(4)8[3R+]P{8,7} offers high dispersion and dissipation accuracy on the linear problem while sacrificing nothing on the nonlinear problem. When comparing 3R+ schemes, for “M” and “C” methods, fifth-order methods appear to be more efficient than fourth-order methods for tolerances less than $\approx 10^{-3}$ to 10^{-4} . Comparing RK5(4)8[3R+]C to the RK5(4)7FC and RK5(4)7FS methods of Dormand and Prince,[19, 20] Table 6 indicates that the low-storage method is nearly as accuracy efficient and viscous stability efficient while being more stability efficient on inviscid problems. In this case, the penalty of low-storage is relatively small. One of the surprises in designing low-storage methods was finding $b_3 = b_4 = 0$ in the RK5(4)8[3R+] methods as well as the RK5(4)7[3R+] method. There are also many other cases of unexpected linear dependencies. We suspect that there is an interesting reason behind the order conditions when certain $a_{ij} = b_j$, but a theory eludes us.

Adding a fourth register to a fifth-order method allows for efficiencies that approach more traditional schemes. For RK5(4)6 schemes, RK5(4)6[4R+]M is arguably better than both of Fehlberg’s methods[26] and that of Dormand and Prince[19] in spite of the loss of three DOF to low storage. The most accurate RK5(4)6 published seems to be that of Papakostas and Papageorgiou with $A^{(6)} = 0.0008694$, 1.4% better $\eta^{(\text{acc})}$ than RK5(4)6[4R+]M ($A^{(6)} = 0.0009449$). Sharp[70] offers two RK5(4)6M methods, with $A^{(6)} = 0.0009399$ and $A^{(6)} = 0.0009775$. He also states that the global minima for RK5(4)6 schemes is $A^{(6)} = 0.00087$, consistent with what Papakostas and Papageorgiou have presented. A FSAL method based on RK5(4)6[4R+] type schemes has not been pursued. Moving to seven-stage methods, RK5(4)8[4R+]FM is our only FSAL method. With $A^{(6)} = 0.00003256$, Table 6 suggests that it is 30% more accuracy efficient than the DOPRI5. Efficiencies based on $A^{(7)}$, $A^{(8)}$, and $A^{(9)}$ are even more encouraging. The schemes are would be expected to perform similarly to compared to Sharp and Smart [SS-RK5(4)7]. Papakostas and Papageorgiou recently designed an extremely accurate 5(4) pair [PP-RK5(4)7F] with 6 effective stages. As with the DOPRI5, the disadvantage of this approach relative to fully seven-stage methods is the relatively high values of $A^{(7)}$ and D , and relatively poor linear stability. On paper, the best 5(4) pair appears to be the Bogacki and Shampine [BS-RK5(4)7]. DETEST results show that RK5(4)8[4R+]FM performs as well as or better than SS-RK5(4)7, PP-RK5(4)7F, DOPRI5, or BS-RK5(4)7 while saving two to three registers of memory. These results are slightly controller dependent. The threshold for switching from fourth- to fifth-order 4R+ “M” methods (RK4(3)5[4R+]M and RK5(4)8[4R+]FM) appears to be $\approx 10^{-3}$.

The five-register 5(4) pair RK5(4)7[5R+] is considered to address any $\eta^{(\text{acc})}$ or $A^{(6)}$ shortfall of the 2R, 3R, and 4R 5(4) pairs relative to existing methods. Designing 5(4) methods based on a sixth-order main scheme has been done, first by Sharp and Smart [SS-RK5(4)7] and later by Bogacki and Shampine [BS-RK5(4)7], as well as a $q(q-2)$ -pair by Tsitouras and Papakostas[82] [TP-RK6(4)7]. For the 5(4) pairs $A^{(6)}$ may be set rather arbitrarily, and for these methods $A^{(6)}$ is given by 0.9, 7.1, 2.2, and $0.0(\times 10^{-5})$, respectively. What may be a better measure of the accuracy of these methods is $A^{(7)}$. In the same order, $A^{(7)}$ for these methods is 5.8, 1.8, 2.1, and $2.1(\times 10^{-4})$. Our DETEST results show RK5(4)7[5R+] performing better than DOPRI5, the same as SS-RK5(4)7, and worse than BS-RK5(4)7, PP-RK5(4)7F, and RK5(4)8[4R+]FM.

It is important to consider the benefits of additional registers so that these benefits may be weighed against the cost of the additional memory usage. At fourth order, switching from RK4(3)5[2R+]C to RK4(3)5[3R+]C nets a 6% efficiency gain. For “M” schemes, RK4(3)5[4R+]M is 126% more efficient than RK4(3)5[3R+]M in Table 6. Maximum norm contractivity radius increases 130% by going from

RK4(3)5[3R+]N to RK4(3)5[4R+]N, with an attendant 4% loss in accuracy efficiency. With fifth-order schemes, moving from RK5(4)9[2R+]C to RK5(4)8[3R+]C yields a 12% efficiency gain. Adding registers to RK5(4)9[2R+]M gives a 25% gain with RK5(4)8[3R+]M, 110% with RK5(4)8[4R+]FM, and 160% with RK5(4)7[5R+]M.

Below fifth order there does not appear to be a compelling reason to use full-storage methods. At fifth order, users must establish the cost of memory relative to CPU time to establish the optimal methods. On parallel machines, low-storage methods may enjoy some advantage because of less required communication. When sufficient memory is available and fifth-order accuracy is required, RK5(4)8[4R+]FM is essentially as good as BS-RK5(4)7, SS-RK5(4)7, PP-RK5(4)7F, and RK5(4)7[5R+]M. Low-storage methods will also be relatively more valuable when the number of equations becomes large (i.e. many species). The value increases because the storage required of the integrator is directly proportional to the number of integration variables yet storage for items like grid metrics is not.

Stability plots show that step-control stability is enhanced by switching from an I-controller to a PI-controller in all of the methods presented as well as the reference methods. Whereas with the I-controller schemes are predominantly SC-unstable on their linear stability boundaries, they are predominantly SC-stable with the PI-controller. When methods are SC-unstable with the PI-controller, it is often at either the real axis (viscous) or at the imaginary axis (inviscid), or both. Some room for optimization for each of the methods is possible via α and β . Doing this optimization requires some caution because it is not sufficient in the design of a good controller for each of the eigensolutions to be damped. The time constants associated with these eigensolutions must not be too large or too small. We do not pursue this optimization. Possibly a PID-controller could find use in certain DNS runs. Coping with SC-instability is probably best accomplished by reducing step sizes. In cases where $A^{(q+2)}/A^{(q+1)} \gg 1$, a PI-controller was found to make error control more reliable. Surprisingly, RK4(3)5[4R+]M with $A^{(6)}/A^{(5)} = 130$ was reliable on DETEST with both I- and PI-controllers. In most cases DETEST was able to run at more lax tolerances with the PI-controller than the I-controller. All low-storage schemes were able to run at tolerances as lax as 10^{-1} to 10^{-2} , except RK4(3)5[3R+]M, which would not run above $10^{-2.5}$ with the PI-controller. BS-RK5(4)7 had the worst behavior in this regard, possibly because $R(z)$ and $\hat{R}(z)$ are so similar. With the I-controller, DOPRI5, BS-RK5(4)7, and RK5(4)7[5R+]M, especially the last two, had difficulty at lax tolerances.

Linear advection of information along characteristics is often used as a model problem for studying the hyperbolic limit of the Navier-Stokes equations. An extremely difficult test case is the advection of information over long distances, because it tests both the spatial and temporal resolving capabilities of a scheme. We formulate this test problem with the model equation $\partial U/\partial t + \partial U/\partial x = 0$, solved on the interval $-50 \leq x \leq 450$. The initial and exact solutions are given by the expression $U(x, t) = \frac{1}{2} \exp[-(\frac{x-t}{3})^2]$. The exact solution is a wave packet of energy, spread over an interval approximately six units wide, moving with unit velocity in time. Note that this test case has information content at all wavenumbers. The spatial discretization of the first-derivative operator is done with a sixth-order compact operator, known to have adequate spatial resolving capability. The boundary conditions are imposed to ensure that no order reduction occurs.[13]

Figure 7.6 shows linear advection results, obtained with four temporal operators at three spatial resolutions. The logarithm of the global error is plotted as a function of the work. We assume that the spatial resolution dictates the desired accuracy level in the calculation, and that spatial and temporal error components should be approximately equal. Note that as the time-step is decreased (increasing work), all formulations asymptote to a uniform error that corresponds to the spatial operator component. At coarse

error tolerances (six grid points resolving the wave packet), the CFL condition (temporal stability constraint) of all schemes produces temporal and spatial error components that are nearly matched. The fifth-order schemes have no apparent advantage over the fourth-order formulations. At moderate and fine error tolerances (12 and 24 four points), the fifth-order formulations become more efficient. The larger CFL condition of the fourth-order scheme allows a larger time step, but produces inadequate temporal resolutions.

To choose a scheme for a DNS run, all of this information must be sorted. First must be established the relative cost of memory to CPU time in relation to the CPU and memory requirements of the run. The next step is to establish whether the simulation will be more stability bound or accuracy bound. Stability bound simulations favor “C” or “S” methods and the 4(3) pairs. For accuracy bound problems, “M” methods are probably best, and 5(4) pairs for tighter tolerances. For runs where nonlinear stability is deemed important, “N” methods should be used. Acoustic or temporally periodic problems might best use “P” methods. Ultimately, $\eta^{(\text{acc})}$ and $\eta^{(\text{stab})}$ are the most important quantities. DETEST quantifies $\eta^{(\text{acc})}$ nicely, independent of order-of-accuracy, while λ/s and λ_v/s quantify $\eta^{(\text{stab})}$ well. An interesting strategy for users may be to choose an acceptable number of registers and then switch between methods of the same storage requirements. For instance, at three registers one could use RK4(3)5[3R+]C when stability dictates the time step and then switch to RK5(4)8[3R+]C as accuracy becomes more important. When accuracy is paramount RK5(4)8[3R+]M could be used. On stability dominated problems, the general shape of the stability domain in terms of (λ, λ_v) may be loosely inferred from the stability plots in terms of z . For the sixth-order, tridiagonal derivative operator, the axes on the stability plots may be replaced with $\Im(z)/2 \approx \lambda$ and $-\Re(z)/4 \approx \lambda_v$. This guideline can be misleading at the imaginary axis. What tolerance should be used for a DNS run? Given the second sentence in the introduction to this paper, atleast 10^{-3} would seem appropriate. This value also depends on the spatial tolerance, as well as the demands of the phenomena we are attempting to resolve. Lax spatial tolerances will negate tight temporal error tolerances.

It is also useful to consider the effects of simplifying assumptions. Experience in the literature[60] suggests that the best schemes are found by using the minimum number of simplifying assumptions. Our experience with RK5(4)6[4R+] and RK5(4)7[4R+] shows that as long as the embedded method can be designed, using $C(2)$ will reduce $A^{(6)}$ substantially over $C(3)$. Assumption $D(1)$ did not appear to have as dramatic an effect. Judging from RK5(4)8[4R+]FM, it is not unreasonable to think that both BS-RK5(4)7 and RK5(4)7[5R+]M could be improved upon slightly by using only $C(2)$. RK5(4)8[3R+] methods are not possible using $C(3)$. RK5(4)s[2R+] methods have been designed in 9 stages with no simplifying assumptions but would require 10 with $D(1)$ and 12 with $C(2)$. Adding an extra stage to the minimum number necessary for a $q(p)$ pair also appears to be beneficial.[72]

To demonstrate the usefulness of the methods, both RK4(3)5[2R+]C and RK5(4)9[2R+]S have been applied to the DNS of a heated, planar, compressible air jet as well as to methane-air, methanol-air, and hydrogen-air flames. We remark that these choices were made long before many of the other schemes here were created. In the case of the jet, observing sound generation from the flowfield might be useful. Detecting this sound is nontrivial numerically and requires selection of a variable that noticeably manifests acoustic waves traversing the media. Figure 7.7 shows the volumetric acceleration in this jet flow and the sound waves coming off the jet column and leaving the vortical structures.

Considering an infinitesimal, spherical material volume element, dV , the volumetric acceleration is given by $(3/dr)(D^2 dr/Dt^2)$ where dr is the infinitesimal radius of the sphere. Figures 7.8 and 7.9 show the corresponding vortical and temperature fields.

An important question in each simulation is at what tolerance does the order-reduction from boundary

error show itself. Users seeking tight tolerances would be well advised to consult the literature for known solutions to this problem. It may be that hybrid step-controllers similar to the PI- and PID-controllers in combination with those for $q(q-2)$ pairs[82] could add reliability. It would also be very useful to establish the stability contours that correspond to $r_{\mathcal{F}_\infty}$, $r_{\mathcal{F}_2}$, and $r_{\mathcal{L}_\infty}$, because comparing $r_{\mathcal{L}_2}$ to the region of $|R(z)| = 1$ shows that $r_{\mathcal{L}_2}$ is terribly conservative. It grossly underestimates stability on hyperbolic problems. Two of these contours would require determining the absolute monotonicity of a polynomial, $R(z)$ or $K(z)$, with a complex argument.

8. Conclusions. The derivation of low-storage, explicit Runge-Kutta (ERK) schemes has been performed in the context of integrating the compressible Navier-Stokes equations via direct numerical simulation (DNS). Unlike previous derivations of ERK schemes which focus on only a few characteristics, we attempt to optimize methods across a broad range of properties, subject to varying degrees of memory economization. With a storage reduction methodology introduced by van der Houwen and Wray, schemes are optimized for stability and accuracy efficiency, linear and nonlinear stability, error control reliability, step change stability, and dissipation/dispersion accuracy. The methods in this paper may be reasonably expected to span the range of needs for compressible DNS when numerical stiffness is not an issue.

Sixteen ERK pairs are presented using from two to five registers of memory per equation, per grid point, and having accuracies from 3(2) to 5(4). All schemes have high-quality error controllers and generally exhibit step change stability when used with a PI-controller. Methods have been tested by means of not only DETEST, but also the 1D wave equation. Two of the methods have been applied to the DNS of a compressible heated jet as well as methane-air and hydrogen-air flames. Derived 3(2) and 4(3) pairs, where few degrees of freedom are sacrificed for low storage, are competitive with existing full-storage methods. Generally, 4(3) pairs are more accuracy and stability efficient than 3(2) pairs. When stability efficiency is paramount, certain 4(3) pairs are best. For accuracy limited problems, 5(4) pairs are more efficient than 4(3) pairs as tolerances drop below 10^{-3} to 10^{-5} . The transition error tolerance for this switching depends on how many registers are being considered. Although a substantial efficiency penalty accompanies use of 2R and 3R fifth-order methods because of the enormous number of forfeited degrees of freedom, state-of-the-art full-storage methods can be nearly matched while still saving two to three registers of memory. Ultimately, the data presented here should help users determine which method is most appropriate based on the properties most valued and the relative cost of the CPU time to memory usage. Users will need to decide which properties are most valued, make a determination of the relative cost of CPU time to memory, and then choose the appropriate method.

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Appendix A. Implementation of the van der Houwen scheme.

A.1. Two registers. We now consider the details of implementing a five-stage explicit Runge-Kutta method with the van der Houwen methodology for the integration of

$$(A1) \quad \frac{dU}{dt} = F(t, U(t)),$$

from time step n to time step $n + 1$ with only two storage registers. It is understood that U be comprises R variables. Third and fourth registers may be used to store an error estimator and the starting U -vector. Assume register 1 ($R1$) contains the U -vector at time $t^{(n)} = t^{(1)}$, $U^{(n)} = U^{(1)}$. The function $F(U^{(n)}, t^{(n)}) = F^{(n)} = F^{(1)}$ is evaluated and the result is placed in register 2 ($R2$). We now perform the operations (error estimation and retention of $U^{(n)}$ are optional)

$$(A2) \quad \begin{aligned} R_{\text{old}} &= R1 \\ R_{\text{err}} &= (b_1 - \hat{b}_1)(\Delta t)R2 \\ R1 &= R1 + a_{21}(\Delta t)R2 \\ R2 &= R1 + (b_1 - a_{21})(\Delta t)R2, \end{aligned}$$

which translate to

$$(A3) \quad \begin{aligned} R_{\text{old}} &= U^{(n)} \\ R_{\text{err}} &= (b_1 - \hat{b}_1)(\Delta t)F^{(n)} \\ U^{(2)} &= U^{(n)} + a_{21}(\Delta t)F^{(n)} \\ X^{(2)} &= U^{(2)} + (b_1 - a_{21})(\Delta t)F^{(n)} \\ &= U^{(n)} + b_1(\Delta t)F^{(n)}, \end{aligned}$$

where the X -vector is an intermediate vector that is used to pass information from one stage to the next. Boundary conditions for the $U^{(i)}$ -vector are evaluated at $t^{(i)} = t^{(n)} + c_i(\Delta t)$. This constitutes the end of stage 1. The function is now evaluated with the contents of $R1$ and the result is then overwritten onto $R1$. With this we compute

$$(A4) \quad \begin{aligned} R_{\text{err}} &= R_{\text{err}} + (b_2 - \hat{b}_2)(\Delta t)R1 \\ R2 &= R2 + a_{32}(\Delta t)R1 \\ R1 &= R2 + (b_2 - a_{32})(\Delta t)R1, \end{aligned}$$

or

$$(A5) \quad \begin{aligned} R_{\text{err}} &= R_{\text{err}} + (b_2 - \hat{b}_2)(\Delta t)F^{(2)} \\ &= (b_2 - \hat{b}_2)(\Delta t)F^{(2)} + (b_1 - \hat{b}_1)(\Delta t)F^{(n)} \\ U^{(3)} &= X^{(2)} + a_{32}(\Delta t)F^{(2)} \\ &= U^{(n)} + a_{32}(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)} \\ X^{(3)} &= U^{(3)} + (b_2 - a_{32})(\Delta t)F^{(2)} \\ &= U^{(n)} + b_2(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)}. \end{aligned}$$

Stage two is complete. Stage 3 begins with the evaluation of the function with the contents of R2. Overwriting the contents of R2, $U^{(3)}$, with the result of the function evaluation, $F^{(3)}$,

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_3 - \hat{b}_3)(\Delta t)R2 \\
R1 &= R1 + a_{43}(\Delta t)R2 \\
R2 &= R1 + (b_3 - a_{43})(\Delta t)R2,
\end{aligned}
\tag{A6}$$

giving

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_3 - \hat{b}_3)(\Delta t)F^{(3)} \\
&= (b_3 - \hat{b}_3)(\Delta t)F^{(3)} + (b_2 - \hat{b}_2)(\Delta t)F^{(2)} + (b_1 - \hat{b}_1)(\Delta t)F^{(n)} \\
U^{(4)} &= X^{(3)} + a_{43}(\Delta t)F^{(3)} \\
&= U^{(n)} + a_{43}(\Delta t)F^{(3)} + b_2(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)} \\
X^{(4)} &= U^{(4)} + (b_3 - a_{43})(\Delta t)F^{(3)} \\
&= U^{(n)} + b_3(\Delta t)F^{(3)} + b_2(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)}.
\end{aligned}
\tag{A7}$$

To begin stage 4, the function is now evaluated with the contents of R1 and the result is then overwritten into R1. Hence,

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_4 - \hat{b}_4)(\Delta t)R1 \\
R2 &= R2 + a_{54}(\Delta t)R1 \\
R1 &= R2 + (b_4 - a_{54})(\Delta t)R1,
\end{aligned}
\tag{A8}$$

or

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_4 - \hat{b}_4)(\Delta t)F^{(4)} \\
&= (b_4 - \hat{b}_4)(\Delta t)F^{(4)} + (b_3 - \hat{b}_3)(\Delta t)F^{(3)} \\
&\quad + (b_2 - \hat{b}_2)(\Delta t)F^{(2)} + (b_1 - \hat{b}_1)(\Delta t)F^{(n)} \\
U^{(5)} &= X^{(4)} + a_{54}(\Delta t)F^{(4)} \\
&= U^{(n)} + a_{54}(\Delta t)F^{(4)} + b_3(\Delta t)F^{(3)} + b_2(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)} \\
X^{(5)} &= U^{(5)} + (b_4 - a_{54})(\Delta t)F^{(4)} \\
&= U^{(n)} + b_4(\Delta t)F^{(4)} + b_3(\Delta t)F^{(3)} + b_2(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)}.
\end{aligned}
\tag{A9}$$

Stage four is finished. On the final stage, stage 5, the evaluation of the function is done with the contents of R2. Overwriting the contents of R2 with the result of the function evaluation, we finally arrive at

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_5 - \hat{b}_5)(\Delta t)R2 \\
R1 &= R1 + b_5(\Delta t)R2,
\end{aligned}
\tag{A10}$$

or

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_5 - \hat{b}_5)(\Delta t)F^{(5)} \\
&= (b_5 - \hat{b}_5)(\Delta t)F^{(5)} + (b_4 - \hat{b}_4)(\Delta t)F^{(4)} + (b_3 - \hat{b}_3)(\Delta t)F^{(3)} \\
&\quad + (b_2 - \hat{b}_2)(\Delta t)F^{(2)} + (b_1 - \hat{b}_1)(\Delta t)F^{(n)}
\end{aligned}$$

$$\begin{aligned}
U^{(n+1)} &= X^{(5)} + b_5(\Delta t)F^{(5)} \\
&= U^{(n)} + b_5(\Delta t)F^{(5)} + b_4(\Delta t)F^{(4)} + b_3(\Delta t)F^{(3)} + b_2(\Delta t)F^{(2)} + b_1(\Delta t)F^{(n)},
\end{aligned}
\tag{A11}$$

where $t^{(n+1)} = t^{(n)} + (\Delta t)$. It may be desirable to write $U^{(n+1)}$ back into the register that contained $U^{(n)}$ at the beginning of the time step in cases where the scheme has an even number of stages. If a FSAL scheme is being used, then $U^{(n+1)}$ is used to compute $F^{(n+1)}$ and

$$R_{\text{err}} = R_{\text{err}} + (0 - \hat{b}_6)(\Delta t)R1$$

or

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (0 - \hat{b}_6)(\Delta t)F^{(n+1)} \\
&= (0 - \hat{b}_6)(\Delta t)F^{(n+1)} + (b_5 - \hat{b}_5)(\Delta t)F^{(5)} + (b_4 - \hat{b}_4)(\Delta t)F^{(4)} \\
&\quad + (b_3 - \hat{b}_3)(\Delta t)F^{(3)} + (b_2 - \hat{b}_2)(\Delta t)F^{(2)} + (b_1 - \hat{b}_1)(\Delta t)F^{(n)}.
\end{aligned}
\tag{A13}$$

Note that register one has $F^{(n+1)}$ and that if the step is accepted then $F^{(n+1)} = F^{(1)}$ in the new step. To control solution error in a vdH scheme, first some appropriate solution error tolerance is chosen, $\epsilon \approx 10^{-3}$ to 10^{-5} . Then one may determine the $(\Delta t)^{(n+1)}$ based on either the I- or PI- step controller. If $U^{(n+1)}$ and $\hat{U}^{(n+1)}$ are computed to $q = (p + 1)$ -th and p -th order accuracy, respectively, then we may define $\delta^{(n+1)}$ at time $n + 1$ as $\delta^{(n+1)} = U^{(n+1)} - \hat{U}^{(n+1)} = R_{\text{err}}$. Then $\delta^{(n+1)}$ is a local truncation error estimate for the lower order formula. It is also wise to place a limit on how quickly the time step is allowed to increase, factors of between 2 and 5 being the maximum.[69]

A unique problem of the vdH schemes is that if R_{old} is not employed, then when a step size is taken that exceeds the error tolerance it is too late to correct matters. In this case, more conservative values of the “safety factor” κ might be advised. Normally $\kappa = 0.9$ is chosen, but this might be reduced slightly here. Alternatively, the error tolerance, ϵ , could be reduced so that any transgressions of the reduced tolerance might not be a transgression of the original tolerance. It should also be remembered that this procedure makes no sense if the U -vector is not normalized in some way so that meaningful comparisons may be made between, say, the energy equation and the momentum equations. A possible choice would be

$$\delta^{(n+1)*} = \frac{\delta^{(n+1)}}{U^{(n+1)}}$$

in cases where $|U^{(n+1)}|$ is greater than, say, 10^{-8} (depending on machine precision), and where $\delta^{(n+1)*}$ replaces $\delta^{(n+1)}$ in Eq. (2.15) or (2.16).

A.2. Three registers. Extending the vdH concept to allow for three available storage registers for a five-stage, non-FSAL ERK scheme, our discussion follows directly from the 2R case but is more terse. Assume register 1 ($R1$) contains $U^{(n)}$ at time $t^{(n)}$. The function, $F^{(n)}$, is evaluated and the result is placed in register 3 ($R3$). We now perform the operations

$$\begin{aligned}
R_{\text{old}} &= R1 \\
R_{\text{err}} &= (b_1 - \hat{b}_1)(\Delta t)R3 \\
R1 &= R1 + a_{21}(\Delta t)R3 \\
R2 &= R1 + (b_1 - a_{21})(\Delta t)R3,
\end{aligned}
\tag{A15}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_2 - \hat{b}_2)(\Delta t) R1 \\
R2 &= R2 + a_{32}(\Delta t) R1 + (a_{31} - b_1)(\Delta t) R3 \\
R3 &= R2 + (b_2 - a_{32})(\Delta t) R1 + (b_1 - a_{31})(\Delta t) R3,
\end{aligned}
\tag{A16}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_3 - \hat{b}_3)(\Delta t) R2 \\
R3 &= R3 + a_{43}(\Delta t) R2 + (a_{42} - b_2)(\Delta t) R1 \\
R1 &= R3 + (b_3 - a_{43})(\Delta t) R2 + (b_2 - a_{42})(\Delta t) R1,
\end{aligned}
\tag{A17}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_4 - \hat{b}_4)(\Delta t) R3 \\
R1 &= R1 + a_{54}(\Delta t) R3 + (a_{53} - b_3)(\Delta t) R2 \\
R2 &= R1 + (b_4 - a_{54})(\Delta t) R3 + (b_3 - a_{53})(\Delta t) R2,
\end{aligned}
\tag{A18}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_5 - \hat{b}_5)(\Delta t) R1 \\
R2 &= R2 + b_5(\Delta t) R1.
\end{aligned}
\tag{A19}$$

A.3. Four registers.

$$\begin{aligned}
R_{\text{old}} &= R1 \\
R_{\text{err}} &= (b_1 - \hat{b}_1)(\Delta t) R4 \\
R1 &= R1 + a_{21}(\Delta t) R4 \\
R2 &= R1 + (b_1 - a_{21})(\Delta t) R4
\end{aligned}
\tag{A20}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_2 - \hat{b}_2)(\Delta t) R1 \\
R2 &= R2 + a_{32}(\Delta t) R1 + (a_{31} - b_1)(\Delta t) R4 \\
R3 &= R2 + (b_2 - a_{32})(\Delta t) R1 + (b_1 - a_{31})(\Delta t) R4
\end{aligned}
\tag{A21}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_3 - \hat{b}_3)(\Delta t) R2 \\
R3 &= R3 + a_{43}(\Delta t) R2 + (a_{42} - b_2)(\Delta t) R1 + (a_{41} - b_1)(\Delta t) R4 \\
R4 &= R3 + (b_3 - a_{43})(\Delta t) R2 + (b_2 - a_{42})(\Delta t) R1 + (b_1 - a_{41})(\Delta t) R4
\end{aligned}
\tag{A22}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_4 - \hat{b}_4)(\Delta t) R2 \\
R4 &= R4 + a_{54}(\Delta t) R3 + (a_{53} - b_3)(\Delta t) R2 + (a_{52} - b_2)(\Delta t) R1 \\
R1 &= R4 + (b_4 - a_{54})(\Delta t) R3 + (b_3 - a_{53})(\Delta t) R2 + (b_2 - a_{52})(\Delta t) R1
\end{aligned}
\tag{A23}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_5 - \hat{b}_5)(\Delta t) R4 \\
R1 &= R1 + b_5(\Delta t) R4
\end{aligned}
\tag{A24}$$

A.4. Five registers.

$$\begin{aligned}
R_{\text{old}} &= R1 \\
R_{\text{err}} &= (b_1 - \hat{b}_1)(\Delta t)R5 \\
R1 &= R1 + a_{21}(\Delta t)R5 \\
(\text{A25}) \quad R2 &= R1 + (b_1 - a_{21})(\Delta t)R5
\end{aligned}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_2 - \hat{b}_2)(\Delta t)R1 \\
R2 &= R2 + a_{32}(\Delta t)R1 + (a_{31} - b_1)(\Delta t)R5 \\
(\text{A26}) \quad R3 &= R2 + (b_2 - a_{32})(\Delta t)R1 + (b_1 - a_{31})(\Delta t)R5
\end{aligned}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_3 - \hat{b}_3)(\Delta t)R2 \\
R3 &= R3 + a_{43}(\Delta t)R2 + (a_{42} - b_2)(\Delta t)R1 + (a_{41} - b_1)(\Delta t)R5 \\
(\text{A27}) \quad R4 &= R3 + (b_3 - a_{43})(\Delta t)R2 + (b_2 - a_{42})(\Delta t)R1 + (b_1 - a_{41})(\Delta t)R5
\end{aligned}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_4 - \hat{b}_4)(\Delta t)R2 \\
R4 &= R4 + a_{54}(\Delta t)R3 + (a_{53} - b_3)(\Delta t)R2 + (a_{52} - b_2)(\Delta t)R1 + (a_{51} - b_1)(\Delta t)R5 \\
R5 &= R4 + (b_4 - a_{54})(\Delta t)R3 + (b_3 - a_{53})(\Delta t)R2 + (b_2 - a_{52})(\Delta t)R1 + (b_1 - a_{51})(\Delta t)R5 \\
(\text{A28})
\end{aligned}$$

$$\begin{aligned}
R_{\text{err}} &= R_{\text{err}} + (b_5 - \hat{b}_5)(\Delta t)R4 \\
(\text{A29}) \quad R5 &= R5 + b_5(\Delta t)R4.
\end{aligned}$$

Appendix B. Explicit Runge-Kutta Order Conditions.

Equations of conditions[19] for various orders of accuracy are found in many places, e.g., §3.4[21]. Higher order conditions may be derived by using **ButcherMath** found in *Mathematica*. [88, 89] To provide completeness in this work, up to sixth order, these conditions given by

$$\begin{aligned}
\tau_1^{(1)} &= \sum_{i=1}^s b_i - \frac{1}{1!} & \tau_1^{(2)} &= \sum_{i=1}^s b_i c_i - \frac{1}{2!} \\
\tau_1^{(3)} &= \frac{1}{2} \sum_{i=1}^s b_i c_i^2 - \frac{1}{3!} & \tau_2^{(3)} &= \sum_{i,j=1}^s b_i a_{ij} c_j - \frac{1}{3!} \\
\tau_1^{(4)} &= \frac{1}{6} \sum_{i=1}^s b_i c_i^3 - \frac{1}{4!} & \tau_2^{(4)} &= \sum_{i,j=1}^s b_i c_i a_{ij} c_j - \frac{3}{4!} \\
\tau_3^{(4)} &= \frac{1}{2} \sum_{i,j=1}^s b_i a_{ij} c_j^2 - \frac{1}{4!} & \tau_4^{(4)} &= \sum_{i,j,k=1}^s b_i a_{ij} a_{jk} c_k - \frac{1}{4!} \\
\tau_1^{(5)} &= \frac{1}{24} \sum_{i=1}^s b_i c_i^4 - \frac{1}{5!} & \tau_2^{(5)} &= \frac{1}{2} \sum_{i,j=1}^s b_i c_i^2 a_{ij} c_j - \frac{6}{5!} \\
\tau_3^{(5)} &= \frac{1}{2} \sum_{i,j=1}^s b_i a_{ij} c_j a_{ik} c_k - \frac{3}{5!} & \tau_4^{(5)} &= \frac{1}{2} \sum_{i,j=1}^s b_i c_i a_{ij} c_j^2 - \frac{4}{5!} \\
\tau_5^{(5)} &= \frac{1}{6} \sum_{i,j=1}^s b_i a_{ij} c_j^3 - \frac{1}{5!} & \tau_6^{(5)} &= \sum_{i,j,k=1}^s b_i c_i a_{ij} a_{jk} c_k - \frac{4}{5!} \\
\tau_7^{(5)} &= \sum_{i,j,k=1}^s b_i a_{ij} c_j a_{jk} c_k - \frac{3}{5!} & \tau_8^{(5)} &= \frac{1}{2} \sum_{i,j,k=1}^s b_i a_{ij} a_{jk} c_k^2 - \frac{1}{5!} \\
\tau_9^{(5)} &= \sum_{i,j,k,l=1}^s b_i a_{ij} a_{jk} a_{kl} c_l - \frac{1}{5!} & \tau_1^{(6)} &= \frac{1}{120} \sum_{i=1}^s b_i c_i^5 - \frac{1}{6!} \\
\tau_2^{(6)} &= \frac{1}{6} \sum_{i,j=1}^s b_i c_i^3 a_{ij} c_j - \frac{10}{6!} & \tau_3^{(6)} &= \frac{1}{2} \sum_{i,j,k=1}^s b_i c_i a_{ij} c_j a_{ik} c_k - \frac{15}{6!} \\
\tau_4^{(6)} &= \frac{1}{4} \sum_{i,j=1}^s b_i c_i^2 a_{ij} c_j^2 - \frac{10}{6!} & \tau_5^{(6)} &= \frac{1}{2} \sum_{i,j,k=1}^s b_i a_{ij} c_j^2 a_{ik} c_k - \frac{10}{6!} \\
\tau_6^{(6)} &= \frac{1}{6} \sum_{i,j=1}^s b_i c_i a_{ij} c_j^3 - \frac{5}{6!} & \tau_7^{(6)} &= \frac{1}{24} \sum_{i=1}^s b_i a_{ij} c_j^4 - \frac{1}{6!} \\
\tau_8^{(6)} &= \frac{1}{2} \sum_{i,j,k=1}^s b_i c_i^2 a_{ij} a_{jk} c_k - \frac{10}{6!} & \tau_9^{(6)} &= \sum_{i,j,k,l=1}^s b_i a_{ij} a_{ik} c_k a_{il} c_l - \frac{10}{6!} \\
\tau_{10}^{(6)} &= \sum_{i,j,k=1}^s b_i c_i a_{ij} c_j a_{jk} c_k - \frac{15}{6!} & \tau_{11}^{(6)} &= \frac{1}{2} \sum_{i,j,k=1}^s b_i a_{ij} c_j^2 a_{jk} c_k - \frac{6}{6!} \\
\tau_{12}^{(6)} &= \frac{1}{2} \sum_{i,j,k,l=1}^s b_i a_{ij} a_{jk} c_k a_{jl} c_l - \frac{3}{6!} & \tau_{13}^{(6)} &= \frac{1}{2} \sum_{i=1}^s b_i c_i a_{ij} a_{jk} c_k^2 - \frac{5}{6!} \\
\tau_{14}^{(6)} &= \frac{1}{2} \sum_{i,j,k=1}^s b_i a_{ij} c_j a_{jk} c_k^2 - \frac{4}{6!} & \tau_{15}^{(6)} &= \frac{1}{6} \sum_{i,j,k=1}^s b_i a_{ij} a_{jk} c_k^3 - \frac{1}{6!} \\
\tau_{16}^{(6)} &= \sum_{i,j,k,l=1}^s b_i c_i a_{ij} a_{jk} a_{kl} c_l - \frac{5}{6!} & \tau_{17}^{(6)} &= \sum_{i,j,k,l=1}^s b_i a_{ij} c_j a_{jk} a_{kl} c_l - \frac{4}{6!} \\
\tau_{18}^{(6)} &= \sum_{i,j,k,l=1}^s b_i a_{ij} a_{jk} c_k a_{kl} c_l - \frac{3}{6!} & \tau_{19}^{(6)} &= \frac{1}{2} \sum_{i,j,k,l=1}^s b_i a_{ij} a_{jk} a_{kl} c_l^2 - \frac{1}{6!} \\
\tau_{20}^{(6)} &= \sum_{i,j,k,l,m=1}^s b_i a_{ij} a_{jk} a_{kl} a_{lm} c_m - \frac{1}{6!}.
\end{aligned}$$

Verner[86] divides these order conditions into four general categories; quadrature $\tau_1^{(k)}$, $k = 1, 2, 3, 4, 5, 6$; subquadrature $\tau_2^{(3)}$, $\tau_{3,4}^{(4)}$, $\tau_{5,8,9}^{(5)}$, $\tau_{7,15,19,20}^{(6)}$; extended subquadrature $\tau_2^{(4)}$, $\tau_{2,4,6,7}^{(5)}$, $\tau_{2,4,6,8,10,11,13,14,16,17,18}^{(6)}$; and nonlinear $\tau_3^{(5)}$, $\tau_{3,5,9,12}^{(6)}$. Several higher-order “tall-tree” conditions of constraint, important in the design of linear stability, are given by

$$\begin{aligned}
\tau_{48}^{(7)} &= \sum_{i,j,k,l,m,n=1}^s b_i a_{ij} a_{jk} a_{kl} a_{lm} a_{mn} c_n - \frac{1}{7!} \\
\tau_{115}^{(8)} &= \sum_{i,j,k,l,m,n,o=1}^s b_i a_{ij} a_{jk} a_{kl} a_{lm} a_{mn} a_{no} c_o - \frac{1}{8!} \\
\tau_{286}^{(9)} &= \sum_{i,j,k,l,m,n,o,p=1}^s b_i a_{ij} a_{jk} a_{kl} a_{lm} a_{mn} a_{no} a_{op} c_p - \frac{1}{9!}.
\end{aligned}$$

Table 1: Two-register ERK schemes

	RK3(2)4[2R+]C	RK4(3)5[2R+]C	RK5(4)9[2R+]S	RK5(4)9[2R+]C	RK5(4)9[2R+]M
a_{21}	$+\frac{11847461282814}{36547543011857}$	$+\frac{970286171893}{4311952581923}$	$+\frac{1107026461565}{5417078080134}$	$+\frac{2756167973529}{16886029417639}$	$+\frac{5573095071601}{11304125995793}$
a_{32}	$+\frac{3943225443063}{7078155732230}$	$+\frac{6584761158862}{12103376702013}$	$+\frac{38141181049399}{41724347789894}$	$+\frac{11436141375279}{13592993952163}$	$+\frac{315581365608}{4729744040249}$
a_{43}	$-\frac{346793006927}{4029903576067}$	$+\frac{2251764453980}{15575788980749}$	$+\frac{493273079041}{11940823631197}$	$+\frac{88551658327}{2352971381260}$	$+\frac{8734064225157}{30508564569118}$
a_{54}	-	$+\frac{26877169314380}{34165994151039}$	$+\frac{1851571280403}{6147804934346}$	$+\frac{1882111988787}{5590444193957}$	$+\frac{6457785058448}{14982850401353}$
a_{65}	-	-	$+\frac{11782306885191}{62590030070788}$	$+\frac{846820081679}{4754706910573}$	$+\frac{5771559441664}{1818797215013}$
a_{76}	-	-	$+\frac{9452544825720}{13648368537481}$	$+\frac{4475289710031}{6420120086209}$	$+\frac{1906712129266}{6681214991155}$
a_{87}	-	-	$+\frac{4435885630781}{26285702406235}$	$+\frac{1183947748311}{9144450320350}$	$+\frac{311585568784}{2369973437185}$
a_{98}	-	-	$+\frac{2357909744247}{11371140753790}$	$+\frac{3307377157135}{13111544596386}$	$-\frac{4840285693886}{7758383361725}$
b_1	$+\frac{1017324711453}{9774461848756}$	$+\frac{1153189308089}{22510343858157}$	$+\frac{2274579626619}{23610510767302}$	$+\frac{1051460336009}{14326298067773}$	$+\frac{549666665015}{5899839355879}$
b_2	$+\frac{8237718856693}{13685301971492}$	$+\frac{1772645290293}{4653164025191}$	$+\frac{693987741272}{12394497460941}$	$+\frac{930517604889}{7067438519321}$	$-\frac{548816778320}{9402908589133}$
b_3	$+\frac{57731312506979}{19404895981398}$	$-\frac{1672844663538}{4480602732383}$	$-\frac{347131529483}{15096185902911}$	$-\frac{311910530565}{11769786407153}$	$+\frac{1672704946363}{13015471661974}$
b_4	$-\frac{101169746363290}{37734290219643}$	$+\frac{2114624349019}{3568978502595}$	$+\frac{1144057200723}{32081666971178}$	$-\frac{410144036239}{7045999268647}$	$+\frac{1025420337373}{5970204766762}$
b_5	-	$+\frac{5198255086312}{14908931495163}$	$+\frac{1562491064753}{11797114684756}$	$+\frac{16692278975653}{83604524739127}$	$+\frac{1524419752016}{6755273790179}$
b_6	-	-	$+\frac{13113619727965}{44346030145118}$	$+\frac{3777666801280}{13181243438959}$	$-\frac{10259399787359}{43440802207630}$
b_7	-	-	$+\frac{393957816125}{7825732611452}$	$+\frac{286682614203}{12966190094317}$	$+\frac{4242280279850}{10722460893763}$
b_8	-	-	$+\frac{720647959663}{6565743875477}$	$+\frac{3296161604512}{22629905347183}$	$+\frac{1887552771913}{6099058196803}$
b_9	-	-	$+\frac{3559252274877}{14424734981077}$	$+\frac{2993490409874}{13266828321767}$	$-\frac{453873186647}{15285235680030}$
\hat{b}_1	$+\frac{15763415370699}{46270243929542}$	$+\frac{1016888040809}{7410784769900}$	$+\frac{266888888871}{3040372307578}$	$+\frac{3189770262221}{35077884776239}$	$+\frac{330911065672}{9937126492277}$
\hat{b}_2	$+\frac{514528521746}{5659431552419}$	$+\frac{11231460423587}{58533540763752}$	$+\frac{34125631160}{2973680843661}$	$+\frac{780043871774}{11919681558467}$	$-\frac{872991930418}{11147305689291}$
\hat{b}_3	$+\frac{27030193851939}{9429696342944}$	$-\frac{1563879915014}{6823010717585}$	$-\frac{653811289250}{9267220972999}$	$-\frac{483824475979}{5387739450692}$	$+\frac{2575378033706}{14439313202205}$
\hat{b}_4	$-\frac{69544964788955}{30262026368149}$	$+\frac{606302364029}{971179775848}$	$+\frac{323544662297}{2461529853637}$	$+\frac{1306553327038}{9528955984871}$	$+\frac{3046892121673}{11013392356255}$
\hat{b}_5	-	$+\frac{1097981568119}{5980877426909}$	$+\frac{1105885670474}{4964345317203}$	$+\frac{6521106697498}{22565577506855}$	$+\frac{1780184658016}{8929499316295}$
\hat{b}_6	-	-	$+\frac{1408484642121}{8758221613943}$	$+\frac{1400555694605}{19784728594468}$	$+\frac{10265149063}{2098741126425}$
\hat{b}_7	-	-	$+\frac{1454774750537}{11112645198328}$	$+\frac{1183541508418}{13436305181271}$	$+\frac{1643090076625}{4891294770654}$
\hat{b}_8	-	-	$+\frac{772137014323}{4386814405182}$	$+\frac{3036254792728}{15493572606329}$	$+\frac{116106750067}{3955800826265}$
\hat{b}_9	-	-	$+\frac{277420604269}{1857595682219}$	$+\frac{638483435745}{4187244659458}$	$+\frac{866868642257}{42331321870877}$

Table 2: Three-register ERK schemes

	RK4(3)5[3R+]C	RK4(3)5[3R+]M	RK4(3)5[3R+]N	RK5(4)8[3R+]C	RK5(4)8[3R+]P{8,7}	RK5(4)8[3R+]M
a_{21}	$+\frac{2365592473904}{8146167614645}$	$+\frac{17396840518954}{49788467287365}$	$+\frac{4745337637855}{22386579876409}$	$+\frac{141236061735}{3636543850841}$	$+\frac{1298271176151}{60748409385661}$	$+\frac{967290102210}{6283494269639}$
a_{32}	$+\frac{4278267785271}{6823155464066}$	$+\frac{21253110367599}{14558944785238}$	$+\frac{6808157035527}{13197844641179}$	$+\frac{7367658691349}{25881828075080}$	$+\frac{14078610000243}{41877490110127}$	$+\frac{852959821520}{5603806251467}$
a_{43}	$+\frac{2789585899612}{8986505720531}$	$+\frac{4293647616769}{14519312872408}$	$+\frac{4367509502613}{10454198590847}$	$+\frac{6185269491390}{13597512850793}$	$+\frac{553998884433}{1150223130613}$	$+\frac{8043261511347}{8583649637008}$
a_{54}	$+\frac{15310836689591}{24358012670437}$	$-\frac{8941886866937}{7464816931160}$	$+\frac{1236962429870}{3429868089329}$	$+\frac{2669739616339}{18583622645114}$	$+\frac{15658478150918}{92423611770207}$	$-\frac{115941139189}{8015933834062}$
a_{65}	-	-	-	$+\frac{42158992267337}{9664249073111}$	$+\frac{18843935397718}{7227975568851}$	$+\frac{2151445634296}{7749920058933}$
a_{76}	-	-	-	$+\frac{970532350048}{4459675494195}$	$+\frac{6206560082614}{27846110321329}$	$+\frac{15619711431787}{74884159414562}$
a_{87}	-	-	-	$+\frac{1415616989537}{7108576874996}$	$+\frac{2841125392315}{14844217636077}$	$+\frac{12444295717883}{11188327299274}$
a_{31}	$-\frac{722262345248}{10870640012513}$	$-\frac{12587430488023}{11977319897242}$	$+\frac{546509042554}{9152262712923}$	$-\frac{343061178215}{2523150225462}$	$-\frac{2491873887327}{11519757507826}$	$+\frac{475331134681}{739607023784}$
a_{42}	$+\frac{1365858020701}{8494387045469}$	$+\frac{6191878339181}{13848262311063}$	$+\frac{625707605167}{5316659119056}$	$-\frac{4057757969325}{18246604264081}$	$-\frac{3833614938189}{14183712281236}$	$-\frac{8677837986029}{16519245648862}$
a_{53}	$+\frac{3819021186}{2763618202291}$	$+\frac{19121624165801}{12321025968027}$	$+\frac{582400652113}{7078426004906}$	$+\frac{1415180642415}{13311741862438}$	$+\frac{628609886693}{8177399110319}$	$+\frac{224500752467}{10812521810777}$
a_{64}	-	-	-	$-\frac{93461894168145}{25333855312294}$	$-\frac{4943723744483}{2558074780976}$	$+\frac{1245361422071}{3717287139065}$
a_{75}	-	-	-	$+\frac{7285104933991}{14106269434317}$	$+\frac{1024000837540}{1998038638351}$	$+\frac{1652079198131}{3788458824028}$
a_{86}	-	-	-	$-\frac{4825949463597}{16828400578907}$	$-\frac{2492809296391}{9064568868273}$	$-\frac{5225103653628}{8584162722535}$
b_1	$+\frac{846876320697}{6523801458457}$	$+\frac{1977388745448}{17714523675943}$	$+\frac{314199625218}{7198350928319}$	$+\frac{514862045033}{4637360145389}$	$+\frac{346820227625}{3124407780749}$	$+\frac{83759458317}{1018970565139}$
b_2	$+\frac{3032295699695}{12397907741132}$	$+\frac{6528140725453}{14879534818174}$	$+\frac{6410344372641}{17000082738695}$	0	0	0
b_3	$+\frac{612618101729}{6534652265123}$	$+\frac{4395900531415}{55649460397719}$	$+\frac{292278564125}{5593752632744}$	0	0	0
b_4	$+\frac{1155491934595}{2954287928812}$	$+\frac{6567440254656}{15757960182571}$	$+\frac{5010207514426}{21876007855139}$	0	0	0
b_5	$+\frac{707644755468}{5028292464395}$	$-\frac{436008689643}{9453681332953}$	$+\frac{5597675544274}{18784428342765}$	$+\frac{2561084526938}{7959061818733}$	$+\frac{814249513470}{2521483007009}$	$+\frac{6968891091250}{16855527649349}$
b_6	-	-	-	$+\frac{4857652849}{7350455163355}$	$+\frac{195246859987}{15831935944600}$	$+\frac{783521911849}{8570887289572}$
b_7	-	-	-	$+\frac{1059943012790}{2822036905401}$	$+\frac{3570596951509}{9788921605312}$	$+\frac{3686104854613}{11232032898210}$
b_8	-	-	-	$+\frac{2987336121747}{15645656703944}$	$+\frac{1886338382073}{9981671730680}$	$+\frac{517396786175}{6104475356879}$
\hat{b}_1	$+\frac{1296459667021}{9516889378644}$	$+\frac{390601394181}{3503051559916}$	$+\frac{1276689330531}{10575835502045}$	$+\frac{1269299456316}{16631323494719}$	$+\frac{679447319381}{8240332772531}$	$-\frac{2632078767757}{9365288548818}$
\hat{b}_2	$+\frac{2599004989233}{11990680747819}$	$+\frac{31150720071161}{68604711794052}$	$+\frac{267542835879}{1241767155676}$	0	0	0
\hat{b}_3	$+\frac{1882083615375}{8481715831096}$	$+\frac{416927665232}{6953044279741}$	$+\frac{1564039648689}{9024646069760}$	$+\frac{2153976949307}{22364028786708}$	$+\frac{798472430005}{13882421602211}$	$+\frac{138832778584802}{30360463697573}$
\hat{b}_4	$+\frac{1577862909606}{5567358792761}$	$+\frac{3879867616328}{8869216637007}$	$+\frac{3243722451631}{13364844673806}$	$+\frac{2303038467735}{18680122447354}$	$+\frac{972791992243}{13597677393897}$	$+\frac{7424139574315}{5603229049946}$
\hat{b}_5	$+\frac{3283349885361}{2316973589007}$	$-\frac{163749046041}{2599987820560}$	$+\frac{606464709716}{2447238536635}$	$+\frac{7354111305649}{15643939971922}$	$+\frac{2994516937385}{6097853295694}$	$-\frac{32993229351515}{6883415042289}$
\hat{b}_6	-	-	-	$+\frac{768474111281}{10081205039574}$	$+\frac{1424705874463}{19211220871144}$	$-\frac{3927384735361}{7982454543710}$
\hat{b}_7	-	-	-	$+\frac{3439095334143}{10786306938509}$	$+\frac{11199564863291}{35136367926059}$	$+\frac{9224293159931}{15708162311543}$
\hat{b}_8	-	-	-	$-\frac{3808726110015}{23644487528593}$	$-\frac{1307718103703}{13694144003901}$	$+\frac{624338737541}{7691046757191}$

Table 3: Four- and five-register ERK schemes

	RK4(3)5[4R+]N	RK4(3)5[4R+]M	RK5(4)6[4R+]M	RK5(4)8[4R+]FM	RK5(4)7[5R+]M
a_{21}	$+\frac{9435338793489}{32856462503258}$	$+\frac{7142524119}{20567653057}$	$+\frac{1811061732419}{6538712036350}$	$+\frac{319960152914}{39034091721739}$	$+\frac{984894634849}{6216792334776}$
a_{32}	$+\frac{6195609865473}{14441396468602}$	$+\frac{20567653057}{89550000000}$	$+\frac{936386506953}{6510757757683}$	$+\frac{16440040368765}{7252463661539}$	$+\frac{984894634849}{5526037630912}$
a_{43}	$+\frac{7502925572378}{28098850972003}$	$+\frac{7407775}{2008982}$	$+\frac{8253430823511}{9903985211908}$	$+\frac{1381950791880}{6599155371617}$	$+\frac{13256335809797}{10977774807827}$
a_{54}	$+\frac{4527781290407}{9280887680514}$	$-\frac{4577300}{867302297}$	$+\frac{4157325866175}{11306150349782}$	$+\frac{18466735994895}{7394178462407}$	$+\frac{5386479425293}{11045691190948}$
a_{65}	-	-	$+\frac{3299942024581}{13404534943033}$	$+\frac{2786140924985}{1426287431161}$	$-\frac{1717767168952}{11602237717369}$
a_{76}	-	-	-	$+\frac{28327099865656}{21470840267743}$	$-\frac{10054679524430}{10306851287569}$
a_{31}	$+\frac{2934593324920}{16923654741811}$	$+\frac{15198616943}{89550000000}$	$+\frac{968127049827}{6993254963231}$	$-\frac{16195115415565}{7808461210678}$	$+\frac{890852251480}{14995156510369}$
a_{42}	$+\frac{16352725096886}{101421723321009}$	$-\frac{226244183627}{80359280000}$	$-\frac{4242729801665}{12001587034923}$	$-\frac{1316066362688}{10261382634081}$	$-\frac{18544705752398}{1842659884027}$
a_{53}	$+\frac{3004243580591}{16885320447374}$	$+\frac{33311687500}{8703531091}$	$+\frac{1960956671631}{3017447659538}$	$-\frac{2389300045797}{9614512377075}$	$+\frac{1115398761892}{28058504699217}$
a_{64}	-	-	$+\frac{2088737530132}{14638867961951}$	$+\frac{6558693593075}{12530787773541}$	$+\frac{5538441135605}{13014942352969}$
a_{75}	-	-	-	$-\frac{5015572218207}{5719938983072}$	$+\frac{23855853001162}{20968156556405}$
a_{41}	$+\frac{390352446067}{5989890148791}$	$+\frac{9890667227}{80359280000}$	$+\frac{332803037697}{7529436905221}$	$+\frac{334167490531}{1677017272502}$	$+\frac{1722683259617}{5669183367476}$
a_{52}	$+\frac{902830387041}{8154716972155}$	$-\frac{20567653057}{6979191486}$	$-\frac{19590089343957}{51581831082203}$	$+\frac{4579492417936}{7930641522963}$	$+\frac{342961171087}{6505721096888}$
a_{63}	-	-	$+\frac{3811366828049}{10653298326636}$	$-\frac{2255846922213}{30066310003000}$	$-\frac{14472869285404}{19736045536601}$
a_{74}	-	-	-	$+\frac{3212719728776}{7037340048693}$	$-\frac{8169744035288}{5424738459363}$
a_{51}	-	-	-	-	$+\frac{762111618422}{5198184381557}$
a_{62}	-	-	-	-	$+\frac{2896263505307}{6364015805096}$
a_{73}	-	-	-	-	$+\frac{60049403517654}{26787923986853}$
b_1	$+\frac{929310922418}{8329727308495}$	$+\frac{297809}{2384418}$	$+\frac{1437717300581}{14622899446031}$	$+\frac{1147876221211}{13910763665259}$	$+\frac{1008141064049}{9867084721348}$
b_2	$+\frac{4343420149496}{15735497610667}$	0	0	0	0
b_3	$+\frac{885252399220}{9490460854667}$	$+\frac{156250000}{270591503}$	$+\frac{3070006287879}{9321175678070}$	$+\frac{182134362610}{9852075053293}$	$+\frac{8222186491841}{18352662300888}$
b_4	$+\frac{3341719902227}{13464012753180}$	$+\frac{5030000}{888933}$	$+\frac{2276970273632}{7940670647385}$	$+\frac{3396705055007}{8495597747463}$	$+\frac{514621697208}{8712119383831}$
b_5	$+\frac{2131913067577}{7868783702050}$	$-\frac{2927}{546}$	$-\frac{1056149936631}{7427907423983}$	$+\frac{363006049056}{2236600357869}$	$+\frac{1808964136873}{4546052443428}$
b_6	-	-	$+\frac{2571845656138}{6012342010435}$	$+\frac{6078825123673}{15200143133108}$	$-\frac{362754645297}{3989911846061}$
b_7	-	-	-	$+\frac{583593328277}{7028929464160}$	$+\frac{599706619333}{7161178965783}$
\hat{b}_1	$+\frac{2929323122013}{17725327880387}$	$+\frac{121286694859}{931793198518}$	$+\frac{399352205828}{2843676810815}$	$+\frac{2023383632057}{26525303340911}$	$+\frac{1633918545125}{12016465907206}$
\hat{b}_2	$+\frac{4379799101587}{35838171763617}$	0	0	0	0
\hat{b}_3	$+\frac{2267325134734}{9725002913543}$	$+\frac{9680751416357}{17201392077364}$	$+\frac{460449895996}{4301836608005}$	$+\frac{480990062147}{12694528747923}$	$+\frac{5614864639673}{10804025076427}$
\hat{b}_4	$+\frac{1519467056643}{8852430786130}$	$+\frac{6633076090000}{1042143269349}$	$+\frac{15965746118666}{21690343195681}$	$+\frac{14502014597821}{36979005529861}$	$+\frac{229286380958}{6920724258831}$
\hat{b}_5	$+\frac{3636375423974}{16547514622827}$	$-\frac{127961558623}{21123456354}$	$-\frac{19281717001664}{29911607353389}$	$-\frac{3883966523914}{63014133260123}$	$+\frac{5960415897193}{14726168927560}$
\hat{b}_6	-	-	$+\frac{5058427127221}{7651806618075}$	$+\frac{1643296191892}{3432451463918}$	$-\frac{4042532386559}{22820216867423}$
\hat{b}_7	-	-	-	$+\frac{2576284903812}{11692468803935}$	$+\frac{930770261899}{11134660916874}$
\hat{b}_8	-	-	-	$-\frac{2393889703871}{16641202878460}$	-

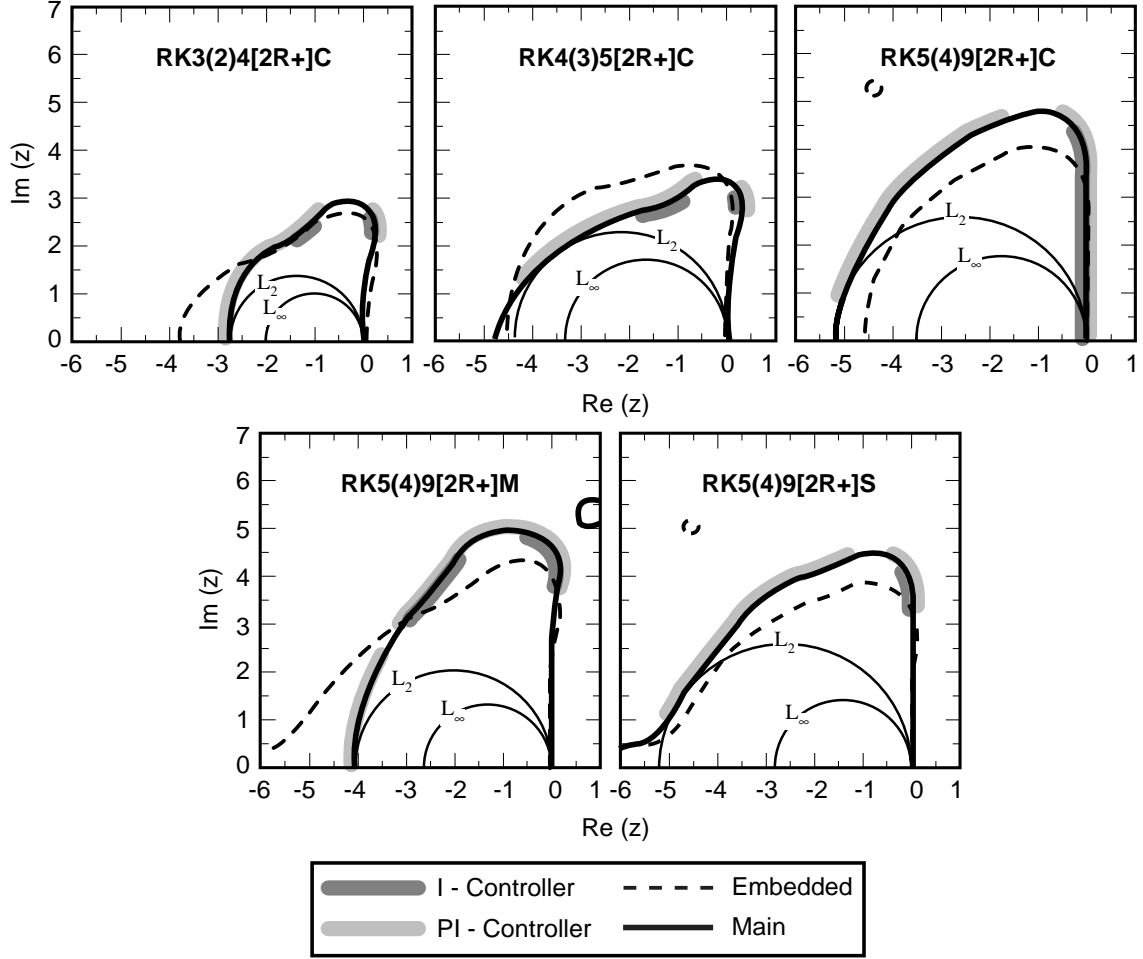


FIG. 3.1. Stability limits of the main and embedded methods for two register schemes, $RK3(2)4[2R+]C$, $RK4(3)5[2R+]C$, $RK5(4)9[2R+]C$, $RK5(4)9[2R+]M$, $RK5(4)9[2R+]S$. Circles denote regions of r_{L_∞} and r_{L_2} contractivity. Shaded regions denote locations along the contour $|R(z)| = 1$ where the methods are SC-stable with either an I- or PI-controller.

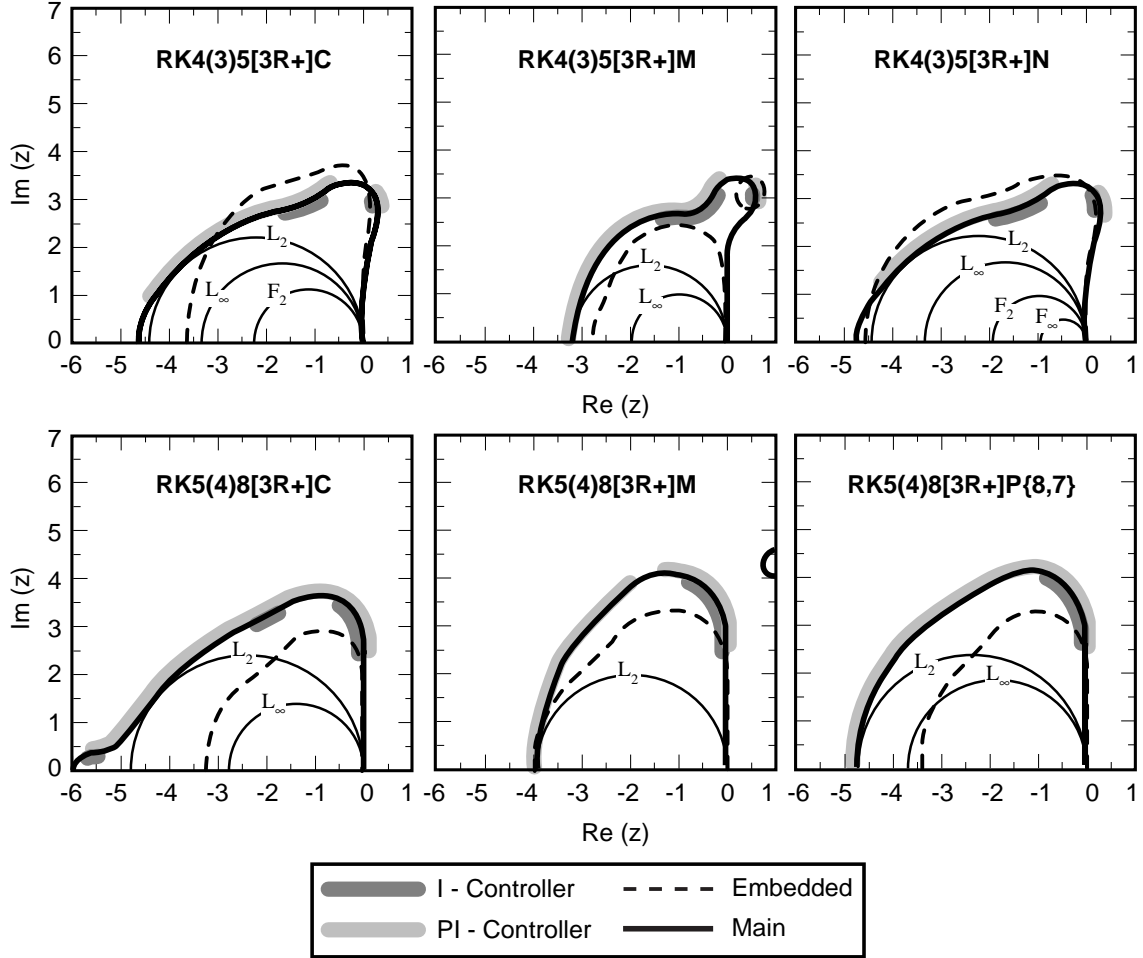


FIG. 4.1. Stability limits of the main and embedded methods for three-register schemes, $RK4(3)5[3R+]C$, $RK4(3)5[3R+]M$, $RK4(3)5[3R+]N$, $RK5(4)8[3R+]C$, $RK5(4)8[3R+]M$, $RK5(4)8[3R+]P\{8,7\}$. Circles denote regions of r_{F_∞} , r_{F_2} , r_{L_∞} , and r_{L_2} contractivity. Shaded regions denote locations along the contour $|R(z)| = 1$ where the methods are SC-stable with either an I- or PI-controller.

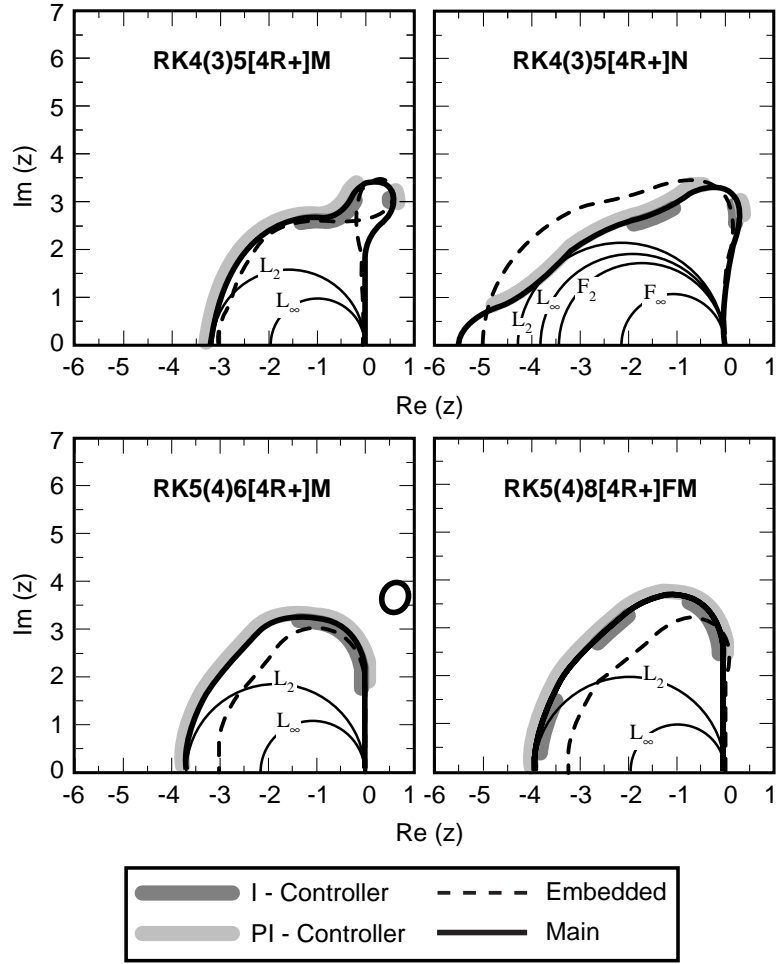


FIG. 5.1. Stability limits of the main and embedded methods for four register schemes, $RK4(3)5[4R+]M$, $RK4(3)5[4R+]N$, $RK5(4)6[4R+]M$, $RK5(4)8[4R+]FM$. Circles denote regions of r_{F_∞} , r_{F_2} , r_{L_∞} , and r_{L_2} contractivity. Shaded regions denote locations along the contour $|R(z)| = 1$ where the methods are SC-stable with either an I- or PI-controller.

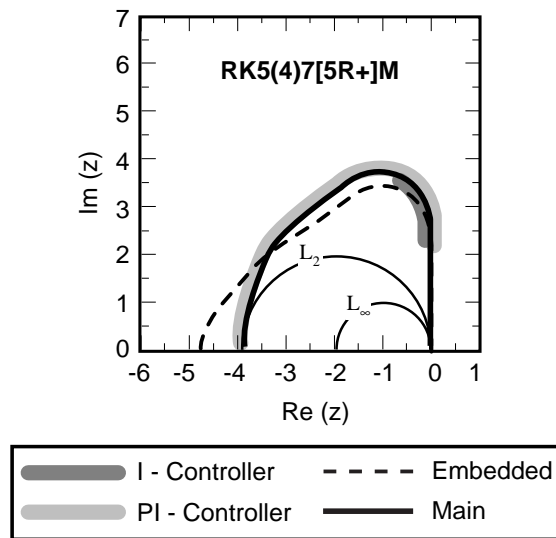


FIG. 6.1. Stability limits of the main and embedded methods for the five-register scheme, $RK5(4)7[5R+]M$. Circles denote regions of $r_{\mathcal{L}_\infty}$ and $r_{\mathcal{L}_2}$ contractivity. Shaded regions denote locations along the contour $|R(z)| = 1$ where the methods are SC-stable using either an I- or PI-controller.

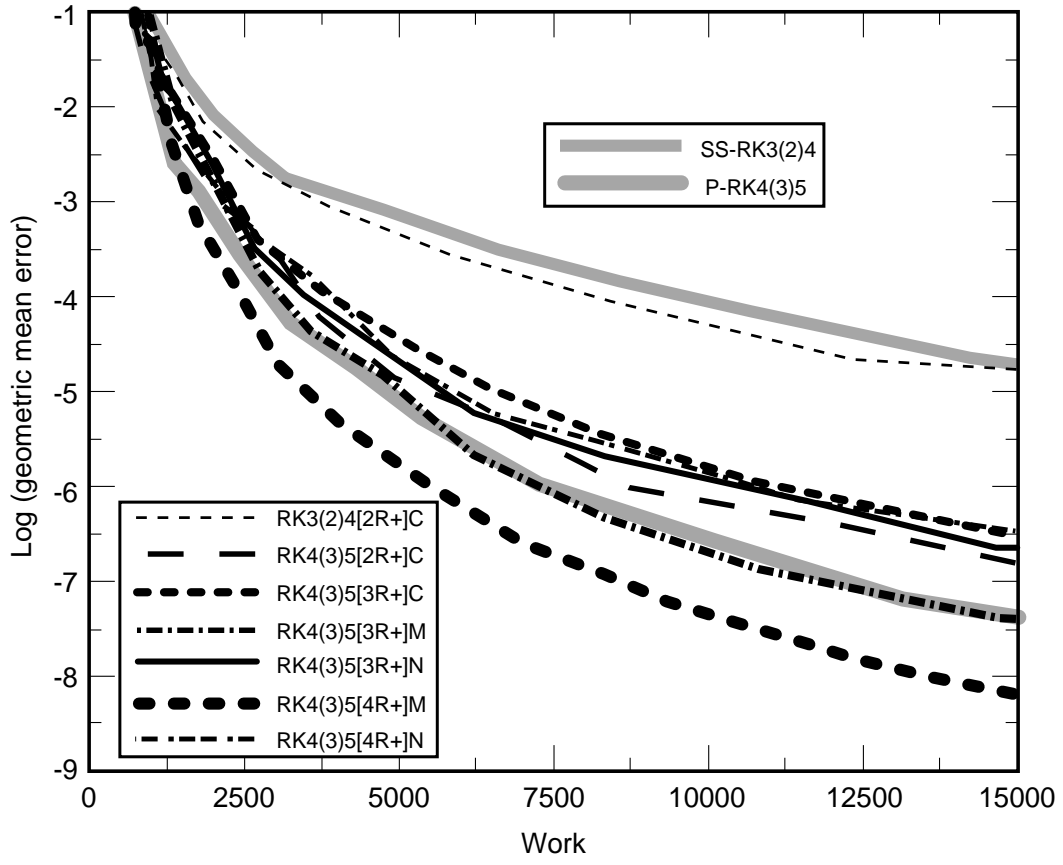


FIG. 7.1. *DETEST* comparison of $3(2)$ and $4(3)$ pairs: low-storage schemes and the reference methods of Sharp and Smart [SS-RK3(2)4] and Prince [P-RK4(3)5].

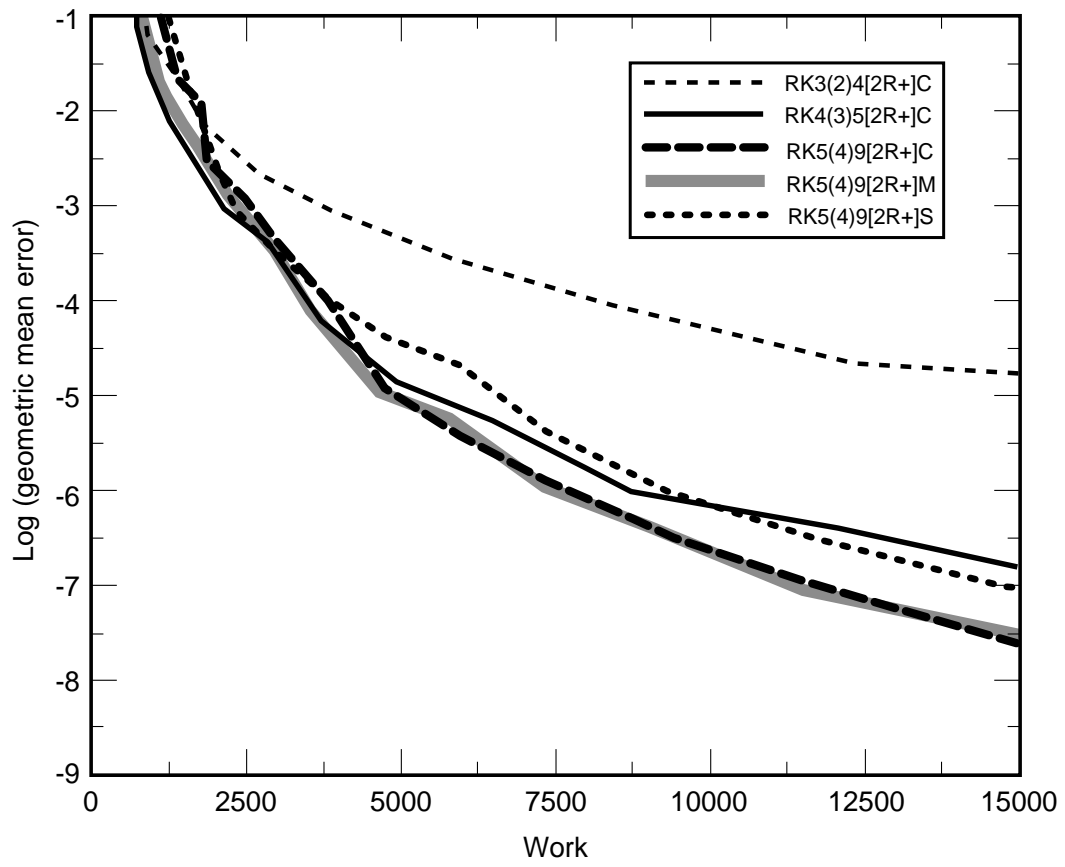


FIG. 7.2. *DETEST* comparison of two-register schemes.

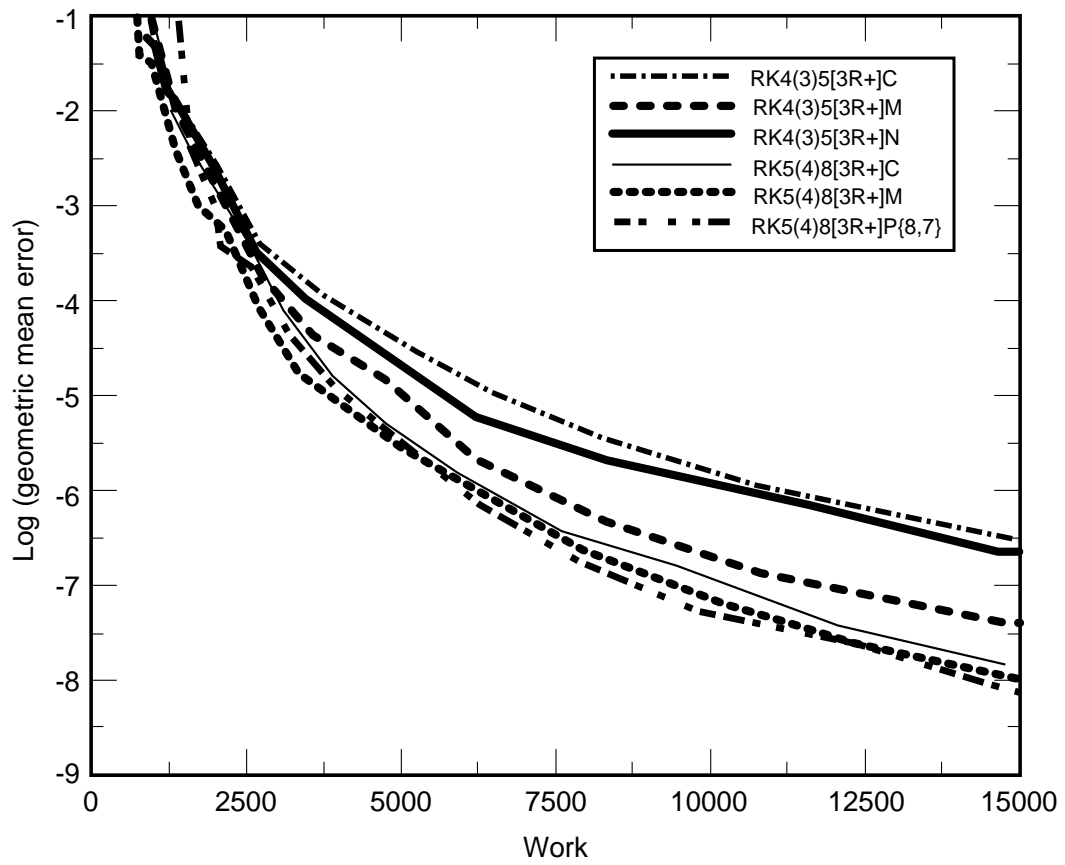


FIG. 7.3. *DETEST* comparison of three-register schemes.

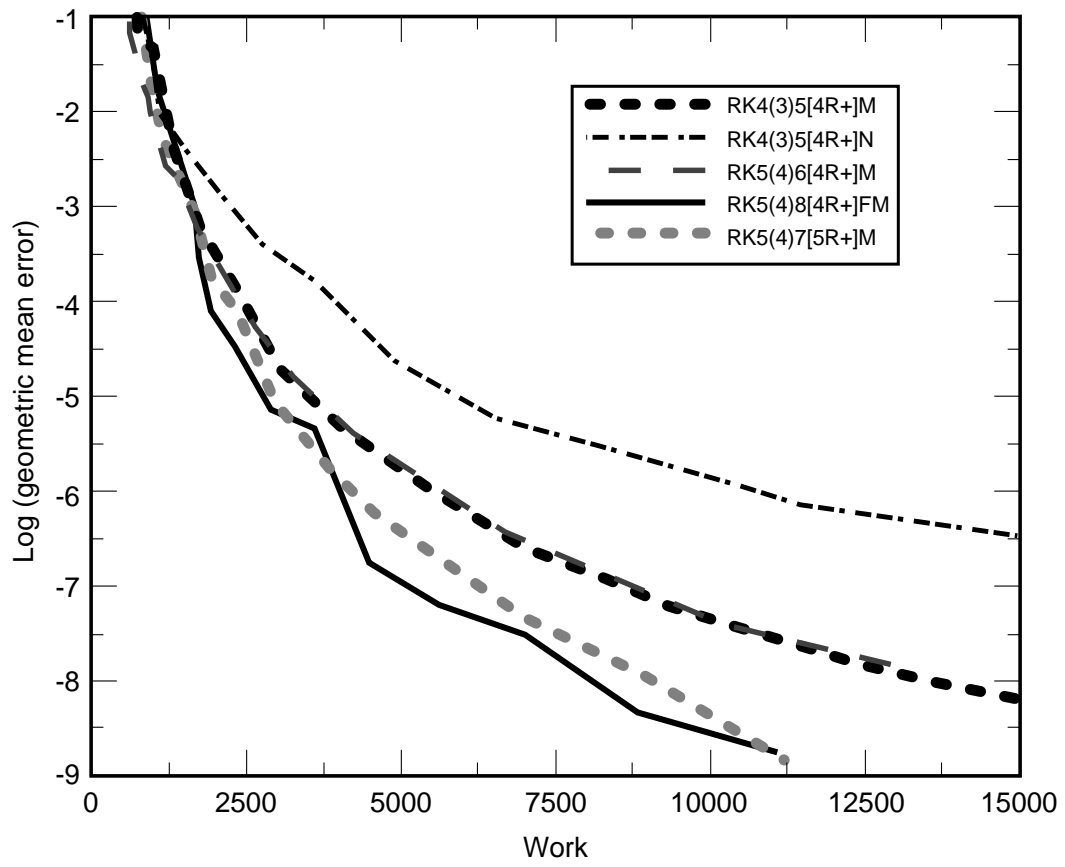


FIG. 7.4. *DETEST* comparison of four- and five-register schemes.

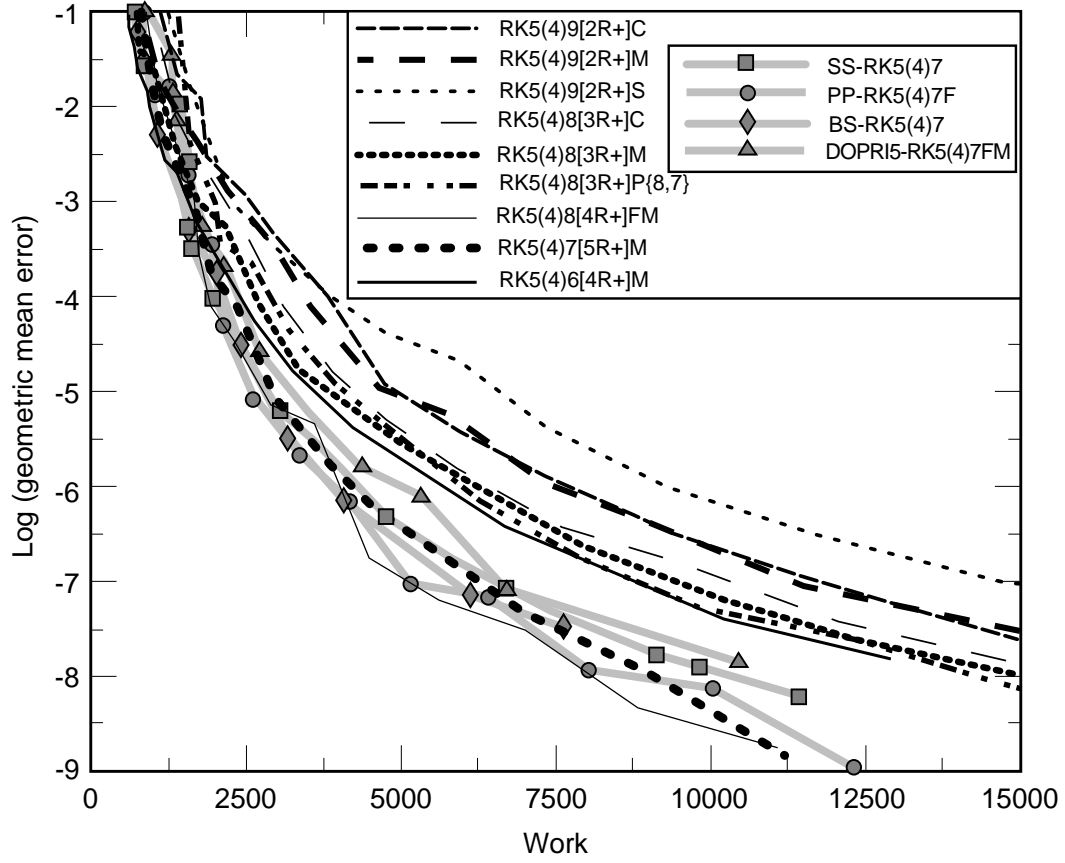


FIG. 7.5. *DETEST* comparison of $5(4)$ pairs: low-storage schemes and the reference methods of Sharp and Smart [$SS-RK5(4)7$], Papakostas and Papageorgiou [$PP-RK5(4)7F$], Bogacki and Shampine [$BS-RK5(4)7$], and Dormand and Prince [$DOPRI5-RK5(4)7FM$].

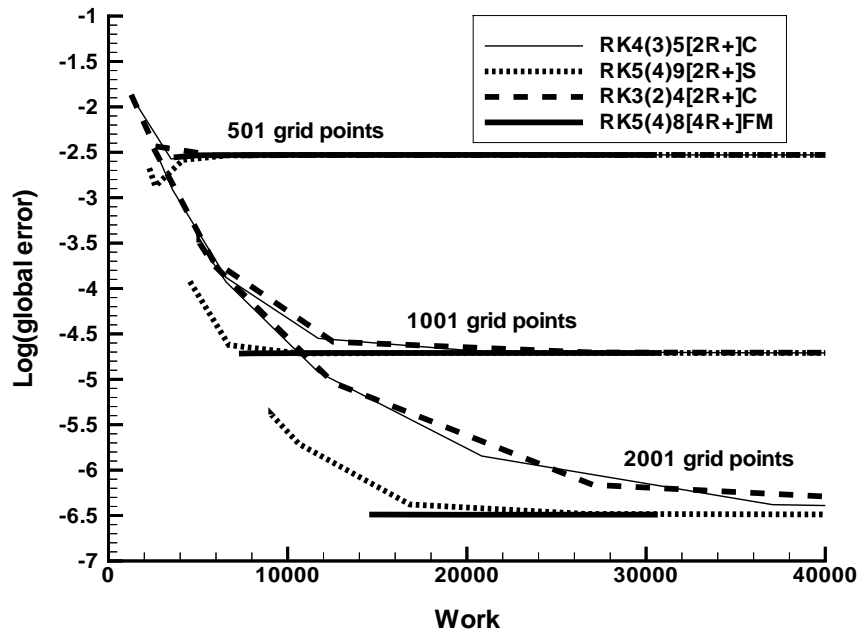


FIG. 7.6. Overall error on $\partial U/\partial t + \partial U/\partial x = 0$ as a function of temporal error tolerance, spatial grid density, and method.

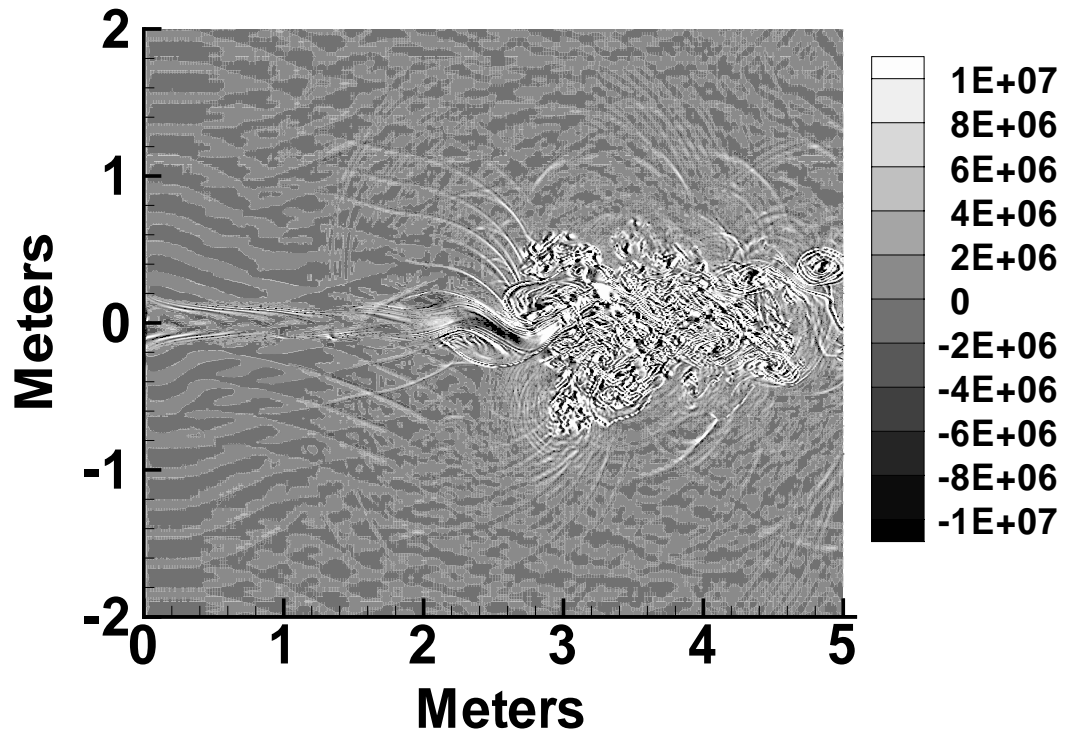


FIG. 7.7. Volumetric acceleration, $\theta_{[2]} = \nabla \cdot \mathbf{a}$ (s^{-2}), for a heated, planar, compressible air jet. The self-similar $\text{Ma}_{\text{jet}} = 0.95$ air jet exhausts into a quiescent body of air. Sound waves are seen emanating from the jet column and vortical region.

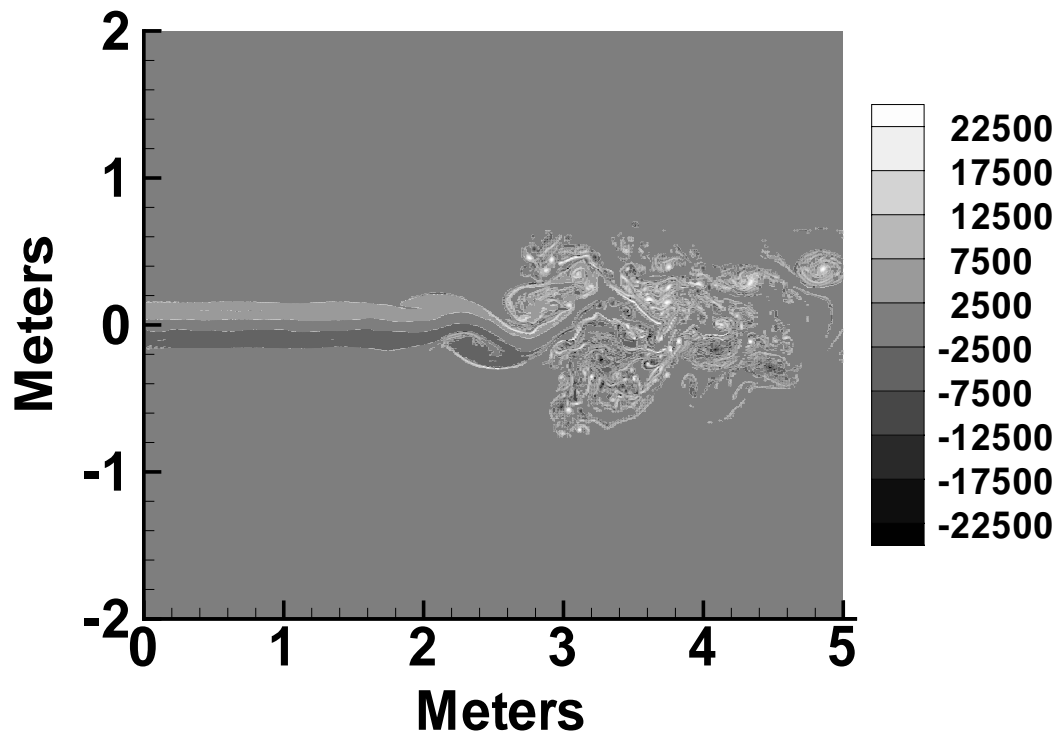


FIG. 7.8. Vorticity, $\nabla \times \mathbf{u}$ (s^{-1}), for a heated, planar, compressible air jet. Large instability growth rates of the high Reynolds number jet give rise to intense regions of vorticity.

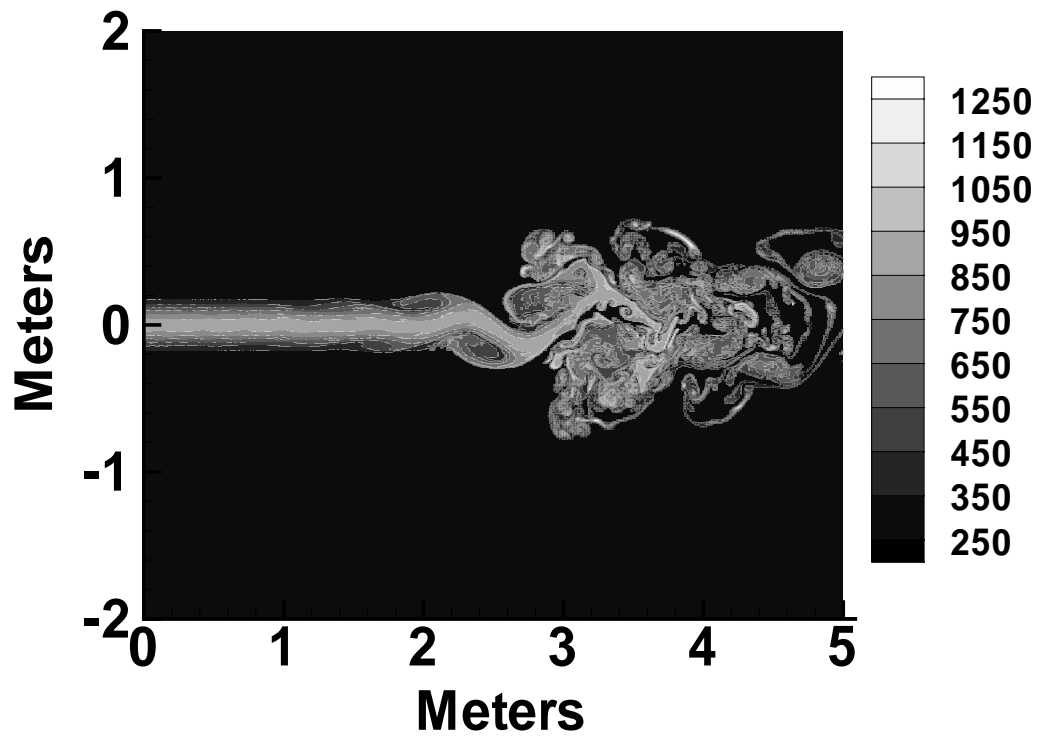


FIG. 7.9. Temperature ($^{\circ}\text{K}$) for a heated, planar, compressible air jet. The $T_{\text{jet}} = 900^{\circ}\text{K}$ air jet rapidly generates finer scale motion due to strong flow instability as it issues into the quiescent $T_{\infty} = 300^{\circ}\text{K}$ air. A Kelvin-Helmholtz instability may be seen in the downstream portion of what remains of the jet column.

Table 4: Third-order ERK schemes: General Characteristics

Author Year	RKq(p)sX	λ λ/s	λ_v λ_v/s	$A^{(q+1)}$ $A_{\infty}^{(q+1)}$	$A^{(q+2)}$ $A_{\infty}^{(q+2)}$	$\eta_{\text{ref}}^{(\text{sec})}$	$\hat{\lambda}$ $\hat{\lambda}/s$	$\hat{\lambda}_v$ $\hat{\lambda}_v/s$	R_s	$\hat{A}^{(p+1)}$ $\hat{A}_{\infty}^{(p+1)}$	$B^{(p+2)}$ $B_{\infty}^{(p+2)}$	$C^{(p+2)}$ $C_{\infty}^{(p+2)}$	D	$E^{(p+2)}$ $E_{\infty}^{(p+2)}$	$\phi(\nu)_{\text{L.O.T.E.}}$ $\alpha(\nu)_{\text{L.O.T.E.}}$	$\tau_{\mathcal{L}_2}, \tau_{\mathcal{L}_{\infty}}, \tau_{\mathcal{F}_2}, \tau_{\mathcal{F}_{\infty}}$ $\hat{\tau}_{\mathcal{L}_2}, \hat{\tau}_{\mathcal{L}_{\infty}}, \hat{\tau}_{\mathcal{F}_2}, \hat{\tau}_{\mathcal{F}_{\infty}}$
Present	RK3(2)4[2R+]C	1.42 0.355	0.70 0.175	1.115(-2) 1.105(-2)	1.312(-2) 8.333(-3)	1.035 -	1.26 0.315	0.97 0.242	0 0	4.051(-2) 3.333(-2)	0.627 0.610	0.542 0.596	2.975	0.275 0.332	$+8.333(-3) \times \nu^5$ $+6.944(-3) \times \nu^6$	1.393, 1.000, 0.000, 0.000 1.726, 1.400, 0.000, 0.000
Sharp et al. 1993	RK3(2)4	1.38 0.345	0.76 0.190	1.280(-2) 8.233(-3)	1.391(-2) 8.333(-3)	1.000 -	1.38 0.345	0.70 0.175	0 0	1.989(-2) 1.583(-2)	1.301 1.467	0.995 0.974	1.219	0.644 0.520	$+3.243(-3) \times \nu^5$ $+5.091(-3) \times \nu^4$	1.513, 1.139, 0.000, 0.000 1.398, 0.977, 0.561, 0.000
Bogacki et al. 1989	RK3(2)4F	0.87 0.218	0.63 0.157	4.181(-2) 4.167(-2)	4.396(-2) 3.333(-2)	0.992	1.12 0.280	0.79 0.198	0 0	2.946(-2) 2.083(-2)	1.349 1.500	1.377 1.500	1.000	1.419 2.000	$-3.333(-2) \times \nu^5$ $+4.167(-2) \times \nu^4$	1.256, 1.000, 0.000, 0.000 1.565, 1.219, 0.958, 0.000
Carpenter et al. 1994	RK3(2)4[2N]	1.41 0.352	0.72 0.180	5.174(-2) 4.863(-2)	4.976(-2) 3.921(-2)	0.705 -	0.07 0.018	0.90 0.225	0 0	6.832(-2) 6.111(-2)	1.143 0.857	1.778 1.653	3.590	0.757 0.796	$+6.565(-3) \times \nu^5$ $+1.768(-3) \times \nu^4$	1.430, 1.044, 0.000, 0.000 1.781, 1.579, 0.000, 0.000
Carpenter et al. 1994	RK3()4[2N]	1.42 0.355	0.70 0.175	7.852(-3) 6.944(-3)	2.805(-2) 2.535(-2)	1.130 -	- -	- -	- -	- -	- -	- -	1.421	- -	$+8.333(-3) \times \nu^5$ $+6.944(-3) \times \nu^6$	1.393, 1.000, 0.620, 0.000 -
Wray 1986	RK3()3[2R]	0.87 0.290	0.63 0.210	4.425(-2) 4.167(-2)	4.587(-2) 3.333(-2)	0.978 -	- -	- -	- -	- -	- -	- -	1.125	- -	$-3.333(-2) \times \nu^5$ $+4.167(-2) \times \nu^4$	1.256, 1.000, 0.000, 0.000 -
Williamson 1980	RK3()3[2N]	0.87 0.290	0.63 0.210	4.398(-2) 4.167(-2)	4.551(-2) 3.333(-2)	0.979 -	- -	- -	- -	- -	- -	- -	1.125	- -	$-3.333(-2) \times \nu^5$ $+4.167(-2) \times \nu^4$	1.256, 1.000, 0.641, 0.000 -
Fehlberg 1969	RK3(2)3	0.87 0.290	0.63 0.210	7.217(-2) 4.167(-2)	5.649(-2) 3.333(-2)	0.865 -	0.04 0.013	0.50 0.167	0 0	1.863(-1) 1.666(-1)	0.775 0.750	0.671 0.250	1.000	0.387 0.250	$-3.333(-2) \times \nu^5$ $+4.167(-2) \times \nu^4$	1.256, 1.000, 1.000, 1.000 1.000, 1.000, 0.000, 0.000
Fehlberg 1969	RK3(2)4F	0.86 0.215	0.62 0.155	5.144(-2) 4.380(-2)	5.317(-2) 3.546(-2)	0.942	0.86 0.215	0.63 0.158	0 0	6.696(-4) 4.735(-4)	72.47 88.00	4.661 1.408	1.000	76.82 92.50	$-3.546(-2) \times \nu^5$ $+4.380(-2) \times \nu^4$	1.232, 0.000, 0.000, 0.000 1.259, 1.003, 0.000, 0.000

Table 5: Fourth-order ERK schemes: General Characteristics

Author Year	$RK(q)p[s]X$	λ λ/s	λ_v λ_v/s	$A_{\infty}^{(q+1)}$ $A_{\infty}^{(q+1)}$	$A_{\infty}^{(q+2)}$ $A_{\infty}^{(q+2)}$	$\eta_{\text{ref}}^{(\text{acc})}$	$\hat{\lambda}$ $\hat{\lambda}/s$	$\hat{\lambda}_v$ $\hat{\lambda}_v/s$	R_z	$\hat{A}_{\infty}^{(p+1)}$ $\hat{A}_{\infty}^{(p+1)}$	$B_{\infty}^{(p+2)}$ $B_{\infty}^{(p+2)}$	$C_{\infty}^{(p+2)}$ $C_{\infty}^{(p+2)}$	D	$E_{\infty}^{(p+2)}$ $E_{\infty}^{(p+2)}$	$\phi(\nu)_{\text{L.O.T.E.}}$ $\alpha(\nu)_{\text{L.O.T.E.}}$	$\tau_{L_2}, \tau_{L_{\infty}}, \tau_{F_2}, \tau_{F_{\infty}}$ $\hat{\tau}_{L_2}, \hat{\tau}_{L_{\infty}}, \hat{\tau}_{F_2}, \hat{\tau}_{F_{\infty}}$
Present	$RK4(3)5[2R+]C$	1.67 0.334	1.21 0.242	5.121(-3) 3.479(-3)	7.447(-3) 2.840(-3)	0.828 -	1.59 0.318	1.13 0.226	0	8.831(-3) 5.952(-3)	1.409 1.026	0.964 0.871	0.845	0.580 0.584	+3.479(-3) \times ν^5 +2.090(-3) \times ν^6	2.229, 1.717, 0.000, 0.000 2.249, 1.860, 0.000, 0.000
Present	$RK4(3)5[3R+]C$	1.67 0.334	1.17 0.234	3.859(-3) 3.333(-3)	4.721(-3) 2.550(-3)	0.876 -	1.75 0.350	0.91 0.182	0	6.492(-3) 5.592(-3)	1.155 0.703	0.808 0.592	1.004	0.594 0.560	+3.333(-3) \times ν^5 +1.944(-3) \times ν^6	2.221, 1.667, 1.129, 0.000 1.820, 1.419, 1.162, 0.000
Present	$RK4(3)5[3R+]M$	0.22 0.044	0.81 0.162	1.884(-3) 1.210(-3)	1.318(-2) 8.530(-3)	1.011 -	0.44 0.088	0.68 0.136	0	7.670(-3) 4.630(-3)	0.977 0.926	1.053 0.974	1.552	0.246 0.261	+1.190(-3) \times ν^7 -1.389(-3) \times ν^6	1.609, 1.000, 0.000, 0.000 1.350, 0.651, 0.000, 0.000
Present	$RK4(3)5[3R+]N$	1.67 0.334	1.20 0.240	4.587(-3) 3.424(-3)	5.917(-3) 2.712(-3)	0.846 -	1.63 0.326	1.15 0.230	0	7.060(-3) 4.846(-3)	1.415 1.030	0.973 0.862	0.864	0.650 0.706	+3.424(-3) \times ν^5 +2.035(-3) \times ν^6	2.228, 1.697, 0.995, 0.477 2.279, 1.814, 1.293, 0.447
Present	$RK4(3)5[4R+]M$	0.22 0.045	0.81 0.163	3.216(-5) 1.692(-5)	4.191(-3) 2.724(-3)	2.283 -	0.49 0.099	0.73 0.147	0	3.431(-3) 3.205(-3)	1.350 1.320	1.354 1.324	6.365	0.009 0.005	+1.250(-5) \times ν^5 -1.376(-3) \times ν^6	1.610, 1.002, 0.000, 0.000 1.448, 0.818, 0.000, 0.000
Present	$RK4(3)5[4R+]N$	1.63 0.326	1.40 0.280	5.635(-3) 3.985(-3)	6.940(-3) 3.410(-3)	0.812 -	1.56 0.312	1.25 0.250	0	8.738(-3) 5.963(-3)	1.307 0.990	0.991 0.917	0.893	0.645 0.668	+3.985(-3) \times ν^5 +2.596(-3) \times ν^6	2.159, 1.916, 1.733, 1.095 2.490, 2.025, 1.620, 1.112
Stanescu et al. 1998	$RK4()6[2N]$	0.83 0.138	0.87 0.145	3.344(-3) 2.596(-3)	3.479(-3) 1.919(-3)	0.751 -	- -	- -	-	- -	- -	- -	1.148	- -	+5.228(-4) \times ν^5 +9.107(-4) \times ν^6	1.734, 0.985, 0.361, 0.000
Carpenter et al. 1994	$RK4()5[2N]$	1.67 0.334	1.17 0.234	4.266(-3) 3.333(-3)	4.905(-3) 2.433(-3)	0.859 -	- -	- -	-	- -	- -	- -	1.027	- -	+3.333(-3) \times ν^5 +1.944(-3) \times ν^6	2.221, 1.667, 0.000, 0.000
Nørsett 1986	$RK4(3)5$	1.42 0.284	0.70 0.140	1.207(-2) 8.333(-3)	1.378(-2) 6.944(-3)	0.698 -	0.87 0.174	0.63 0.126	0	4.330(-2) 4.167(-2)	1.034 0.800	1.146 1.000	1.257	0.279 0.200	+8.333(-3) \times ν^5 +6.944(-3) \times ν^6	1.393, 1.000, 0.000, 0.000 1.256, 1.000, 0.000, 0.000
Prince 1979	$RK4(3)5M$	0.22 0.044	0.81 0.162	1.993(-3) 1.667(-3)	3.222(-3) 1.389(-3)	1.000 -	0.56 0.112	0.62 0.124	0	1.344(-2) 1.250(-2)	0.921 0.800	0.873 0.800	5.000	0.148 0.133	+1.190(-3) \times ν^7 -1.389(-2) \times ν^6	1.609, 1.000, 0.000, 0.000 1.236, 0.467, 0.000, 0.000
Fehlberg(#1) 1969	$RK4(3)5$	1.61 0.322	1.03 0.206	7.142(-3) 4.365(-3)	7.445(-3) 3.260(-3)	0.775 -	0.10 0.020	0.65 0.130	1	6.898(-3) 5.952(-3)	1.818 1.400	1.028 0.278	1.535	1.035 0.733	+4.365(-3) \times ν^5 +2.976(-3) \times ν^6	2.019, 1.642, 0.000, 0.000 1.291, 0.875, 0.000, 0.000
Fehlberg(#2) 1969	$RK4(3)5$	1.53 0.306	0.81 0.162	9.133(-3) 5.775(-3)	9.915(-3) 4.487(-3)	0.738 -	0.11 0.022	0.66 0.132	1	4.556(-3) 4.386(-3)	2.866 2.071	1.007 0.133	1.770	2.005 1.317	+5.775(-3) \times ν^5 +4.386(-3) \times ν^6	1.613, 1.234, 0.000, 0.000 1.315, 0.905, 0.000, 0.000
Zonneveld 1963	$RK4(3)5$	1.42 0.284	0.70 0.140	1.450(-2) 8.333(-3)	1.604(-2) 6.944(-3)	0.672 -	0.06 0.012	0.57 0.114	0	1.443(-1) 1.250(-1)	1.811 1.317	1.768 1.250	5.333	0.100 0.067	+8.333(-3) \times ν^5 +6.944(-3) \times ν^6	1.393, 1.000, 0.000, 0.000 1.137, 0.400, 0.000, 0.000
Merson 1957	$RK4(3)5$	1.74 0.348	0.89 0.178	5.705(-3) 4.167(-3)	7.492(-3) 3.125(-3)	0.810 -	0.22 0.044	0.81 0.162	1	6.481(-3) 5.555(-3)	1.684 1.292	1.185 0.917	2.000	0.880 0.750	+1.389(-3) \times ν^5 +2.894(-4) \times ν^8	1.774, 1.200, 0.000, 0.000 1.609, 1.000, 0.000, 0.000

Table 6: Fifth-order schemes: General Characteristics

Author Year	$RK(q)p \leq X$	λ λ/s	λ_v λ_v/s	$A^{(g+1)}$ $A_\infty^{(g+1)}$	$A^{(g+2)}$ $A_\infty^{(g+2)}$	$\eta_{ref}^{(sc)}$	$\hat{\lambda}$ $\hat{\lambda}/s$	$\hat{\lambda}_v$ $\hat{\lambda}_v/s$	R_s	$\hat{A}^{(p+1)}$ $\hat{A}_\infty^{(p+1)}$	$B^{(p+2)}$ $B_\infty^{(p+2)}$	$C^{(p+2)}$ $C_\infty^{(p+2)}$	D	$E^{(p+2)}$ $E_\infty^{(p+2)}$	$\phi(\nu)_{L.O.T.E.}$ $\alpha(\nu)_{L.O.T.E.}$	$\tau_{L2}, \tau_{L\infty}$ $\hat{\tau}_{L2}, \hat{\tau}_{L\infty}$
Present	$RK5(4)9[2R+]S$	1.78 0.198	1.59 0.177	1.014(-3) 4.869(-4)	1.505(-3) 6.288(-4)	0.411 -	1.60 0.178	1.61 0.179	0	2.121(-3) 1.286(-3)	1.619 1.370	1.399 1.313	1.010	0.478 0.379	-5.159(-5) $\times \nu^7$ +8.439(-5) $\times \nu^6$	2.603, 1.422 2.470, 1.818
Present	$RK5(4)9[2R+]C$	1.05 0.117	1.29 0.144	8.209(-4) 3.868(-4)	1.214(-3) 5.601(-4)	0.426 -	1.63 0.182	1.15 0.128	0	2.031(-3) 1.240(-3)	1.518 1.399	1.278 1.219	1.017	0.404 0.312	-3.258(-5) $\times \nu^7$ +3.609(-5) $\times \nu^6$	2.566, 1.753 2.281, 2.029
Present	$RK5(4)9[2R+]M$	0.31 0.034	1.02 0.113	6.172(-4) 3.096(-4)	1.244(-3) 4.835(-4)	0.447 -	1.97 0.219	1.65 0.183	0	1.895(-3) 1.020(-3)	1.716 1.889	1.453 1.726	0.846	0.326 0.304	-1.555(-4) $\times \nu^7$ -1.856(-4) $\times \nu^6$	2.037, 1.330 2.549, 1.000
Present	$RK5(4)8[3R+]C$	1.31 0.164	1.53 0.191	8.306(-4) 4.013(-4)	1.558(-3) 7.372(-4)	0.478 -	0.92 0.115	0.81 0.101	0	1.377(-3) 6.410(-4)	2.476 2.820	2.283 2.619	4.462	0.603 0.626	-7.791(-5) $\times \nu^7$ +1.736(-4) $\times \nu^6$	2.426, 1.410 1.616, 0.000
Present	$RK5(4)8[3R+]P\{8, 7\}$	1.01 0.126	1.20 0.150	7.923(-4) 3.996(-4)	1.452(-3) 7.729(-4)	0.482 -	1.06 0.133	0.86 0.107	0	1.607(-3) 5.259(-4)	1.902 1.955	1.723 1.772	2.607	0.493 0.432	-9.724(-6) $\times \nu^9$ +1.248(-5) $\times \nu^8$	2.394, 1.853 1.716, 0.000
Present	$RK5(4)8[3R+]M$	0.31 0.039	0.99 0.124	3.240(-4) 1.776(-4)	4.830(-4) 2.360(-4)	0.560 -	0.81 0.101	1.00 0.125	0	3.349(-3) 1.809(-3)	0.905 0.835	0.912 0.838	4.793	0.097 0.098	+1.264(-4) $\times \nu^7$ -1.776(-4) $\times \nu^6$	1.975, 0.000 1.988, 0.000
Present	$RK5(4)6[4R+]M$	0.31 0.053	0.93 0.155	9.449(-4) 5.293(-4)	1.318(-3) 4.678(-4)	0.624 -	0.83 0.139	0.76 0.127	0	3.136(-3) 2.035(-3)	1.286 1.064	1.326 1.088	0.845	0.302 0.260	-9.496(-5) $\times \nu^7$ -1.035(-4) $\times \nu^6$	1.841, 1.080 1.513, 0.645
Present	$RK5(4)8[4R+]FM$	0.99 0.142	0.98 0.140	3.256(-5) 1.863(-5)	2.906(-4) 1.459(-4)	0.938 -	1.27 0.182	0.81 0.117	0	6.571(-4) 4.210(-4)	1.576 1.798	1.563 1.793	2.497	0.050 0.044	+1.058(-5) $\times \nu^7$ -1.044(-6) $\times \nu^6$	1.942, 0.953 1.617, 0.000
Present	$RK5(4)7[5R+]M$	0.92 0.132	0.99 0.142	8.959(-6) 5.000(-6)	5.771(-4) 3.046(-4)	1.163 -	1.05 0.151	1.19 0.171	0	6.583(-4) 4.967(-4)	0.843 0.724	0.851 0.734	2.242	0.014 0.010	+3.194(-6) $\times \nu^7$ -4.937(-7) $\times \nu^6$	1.967, 0.986 2.213, 1.138
Papakostas et al. 1996	$RK5(4)7F$	0.36 0.051	0.89 0.127	6.550(-5) 3.017(-5)	1.693(-3) 9.299(-4)	0.974 -	0.21 0.030	0.87 0.124	0	3.587(-3) 3.072(-3)	1.827 1.195	1.823 1.194	13.74	0.018 0.010	-2.237(-4) $\times \nu^7$ +2.532(-2) $\times \nu^6$	1.763, 0.982 1.730, 1.191
Bogacki et al. 1996	$RK5(4)7$	0.84 0.120	1.00 0.143	2.217(-5) 1.270(-5)	2.126(-4) 9.088(-5)	1.000 -	0.89 0.127	1.02 0.146	0	1.060(-4) 8.371(-5)	1.268 1.043	1.193 0.345	1.164	0.209 0.152	-6.925(-5) $\times \nu^7$ +3.463(-6) $\times \nu^6$	1.994, 1.020 2.024, 1.037
Sharp et al. 1993	$RK5(4)7$	0.91 0.131	0.99 0.141	7.056(-5) 3.475(-5)	1.774(-4) 8.683(-5)	0.825 -	1.00 0.143	1.20 0.172	0	7.814(-4) 6.299(-4)	1.141 0.882	1.132 0.844	1.000	0.090 0.055	+2.488(-5) $\times \nu^7$ -2.633(-5) $\times \nu^6$	1.958, 0.988 2.254, 1.187
Dormand et al. 1986	$RK5(4)7FC$	0.26 0.037	1.12 0.160	1.489(-3) 7.051(-4)	2.064(-3) 9.909(-4)	0.579 -	0.29 0.041	1.09 0.156	0	7.479(-4) 4.808(-4)	2.752 2.647	1.724 1.214	3.603	1.991 1.467	+2.289(-4) $\times \nu^7$ -4.274(-4) $\times \nu^6$	2.218, 1.444 2.168, 1.445
Dormand et al. 1980	$RK5(4)7FM$	0.51 0.073	0.83 0.119	3.991(-4) 2.778(-4)	3.956(-3) 3.735(-3)	0.721 -	0.23 0.033	1.10 0.157	0	1.183(-3) 8.083(-4)	1.542 1.240	1.665 0.987	11.60	0.337 0.344	-4.762(-4) $\times \nu^7$ +2.778(-4) $\times \nu^6$	1.653, 0.833 2.192, 1.327
Dormand et al. 1980	$RK5(4)7FS$	0.25 0.036	1.44 0.206	1.813(-3) 1.029(-3)	2.510(-3) 1.394(-3)	0.560 -	0.24 0.034	1.50 0.214	0	4.207(-4) 2.716(-4)	4.973 4.097	1.743 0.859	3.857	4.310 3.788	-4.189(-4) $\times \nu^7$ -6.173(-4) $\times \nu^6$	2.322, 1.800 2.152, 0.000
Dormand et al. 1980	$RK5(4)6M$	0.31 0.052	0.94 0.157	1.227(-3) 8.333(-4)	1.642(-3) 8.770(-4)	0.598 -	0.22 0.037	0.93 0.155	0	2.227(-3) 1.222(-3)	1.281 1.009	1.344 0.550	3.436	0.551 0.682	-5.952(-5) $\times \nu^7$ -1.389(-4) $\times \nu^6$	1.867, 1.111 1.858, 1.327
Fehlberg(#1) 1969	$RK5(4)6$	0.27 0.045	1.05 0.175	1.448(-3) 6.944(-4)	2.124(-3) 1.155(-3)	0.581 -	0.19 0.032	0.73 0.122	0	3.079(-3) 2.083(-3)	1.772 1.667	1.396 0.792	6.750	0.470 0.333	+1.488(-4) $\times \nu^7$ -3.472(-4) $\times \nu^6$	2.083, 1.333 1.463, 0.800
Fehlberg(#2) 1969	$RK5(4)6$	0.23 0.038	0.92 0.153	3.356(-3) 1.816(-3)	6.765(-3) 3.780(-3)	0.505 -	0.19 0.032	0.76 0.127	0	1.839(-3) 1.282(-1)	3.156 2.590	1.364 0.837	8.000	1.825 1.417	+7.097(-4) $\times \nu^7$ -9.081(-4) $\times \nu^6$	1.839, 1.286 1.510, 0.867